FINAL REPORT

Estimated Exposure and Lifetime Cancer Incidence Risk from Carbon Tetrachloride Released to the Air from the Rocky Flats Plant

Part of Task 3: Independent Analysis of Exposure, Dose, and Health Risk to Offsite Individuals

August 1999

Submitted to the Colorado Department of Public Health and Environment, Disease Control and Environmental Epidemiology Division, Rocky Flats Health Studies in partial fulfillment of Contract No. 100APPRCODE 391

"Setting the standard in environmental health"

RAC

Radiological Assessments Corporation
417 Till Road Neeses, South Carolina 29107
phone 803.536.4883 fax 803.534.1995

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Authors

Patricia D. McGavran, Ph.D., McGavran Toxicology Consulting, Inc.
Arthur S. Rood, K-Spar, Inc.

Principal Investigator

John E Till, Ph.D., *Radiological Assessments Corporation*

EXECUTIVE SUMMARY

The Rocky Flats Environmental Technology Site is owned by the U.S. Department of Energy (DOE) and is currently contractor-operated by Kaiser-Hill Company. For most of its history, the site was called the Rocky Flats Plant (RFP) and was operated by Dow Chemical Company as a nuclear weapons research, development, and production complex. The RFP is located about 8–10 km from the cities of Arvada, Westminster, and Broomfield, Colorado and 26 km (16 mi). northwest of downtown Denver, Colorado.

Through a 1989 Agreement in Principle between the DOE and the State of Colorado, DOE provided the State with funding and technical support for health-related studies. The purpose of the Historical Public Exposures Studies on Rocky Flats is to identify potential health effects in residents in nearby communities who may have been exposed to past toxic and radioactive releases.

This report documents risk calculations for inhalation of carbon tetrachloride in air resulting from routine operational releases at the RFP. The report evaluates environmental monitoring data, discusses evidence of health effects, and describes environmental transport modeling. Estimates of airborne concentrations with uncertainty are provided along with lifetime carcinogenic incidence risk resulting from inhalation of carbon tetrachloride for generic receptor scenarios.

Source Term. The source term and estimated uncertainty for carbon tetrachloride was investigated by McGavran et al. (1996) and used without modification. In general, the entire reported inventories used at the RFP were assumed to be released to the atmosphere. Carbon tetrachloride is a high vapor pressure volatile organic compound and calculations showed almost all the compound that was disposed of on the ground surface (a common disposal practice in the past) would be released to the air. Maximum annual releases were estimated to be between 50 and 200 tons y^{-1} between the years 1958–1969.

Health Hazards of Carbon Tetrachloride. Chronic exposure to carbon tetrachloride has been shown to cause liver cancer in laboratory animals. However, case reports and studies of workers exposed to high levels of carbon tetrachloride are not conclusive. The evidence has led the U.S. Environmental Protection Agency (EPA) to classify carbon tetrachloride as a probable human carcinogen, rather than a known human carcinogen (EPA 1997). The Health Advisory Panel (HAP) at their December 1994 meeting decided liver cancer was the most appropriate endpoint of interest for chronic exposure. The carcinogenic slope factor for carbon tetrachloride was represented by a lognormal distribution having a geometric mean of 2.5×10^{-2} kg d mg^{-1} and a geometric standard deviation of 1.4.

Environmental Transport Modeling. Five atmospheric transport models ranging from a simple straight-line Gaussian plume model to a complex terrain model were evaluated for use in this study (Rood 1997). Models were compared to tracer measurements taken in the winter of 1991 at Rocky Flats. The results of this evaluation indicated no one model clearly outperformed the others. However, the puff trajectory models, RATCHET, TRIAD, and INPUFF2 generally had lower variability and higher correlation to observed values compared to the other models. The RATCHET model was chosen for these calculations because it was particularly well suited for long-term annual-average dispersion estimates and it incorporates spatially varying meteorological and environmental parameters.

The model domain encompassed a 2200 km^2 area (50 km north-south by 44 km east-west). The domain extended 28 km south, 12 km west, 22 km north, and 32 km east from the RFP. Most of the Denver metropolitan area and the city of Boulder were included in the domain. Reliable meteorological data from RFP is lacking before 1984. For this reason, a recent 5-year (1989–94) meteorological data set was used to determine annual average *X*/Q (concentration divided by release rate) values for 2300 receptor locations in the model domain. Meteorological data taken at the Denver Stapleton International Airport during the same period was also incorporated into the simulations. Annual average concentrations for each year were then determined by multiplying the annual release rate by the appropriate *X*/Q value.

Model prediction uncertainty was accounted for through the use of several multiplicative stochastic correction factors that accounted for uncertainty in the dispersion estimate, the meteorology, and deposition and plume depletion. Dispersion uncertainty was based on distributions on predicted-to-observed ratios from field tracer experiments using the Gaussian plume and other models including RATCHET. These values were derived from literature reviews and results from studies specific to this project. Meteorological uncertainty arises because we are using 5 years of meteorological data spanning a recent time period (1989–1993) to define an annual average *X/Q* value that will be applied to all previous years of the assessment period (1952–1989). This correction factor was derived from studies performed for the Fernald Dosimetry Reconstruction Project (Killough et al. 1996) and additional comparisons made at Rocky Flats. Deposition and plume depletion uncertainty factors were calculated using the Monte Carlo sampling features of RATCHET. All correction factors were distributed lognormally and were combined with the source term uncertainty to yield distributions of predicted concentrations at selected receptor locations. Monte Carlo techniques were used to propagate model prediction uncertainty through to the final risk calculations.

Predicted Concentrations. Predicted concentrations east of the plant along Indiana Avenue ranged from 0.2 (5th percentile) to 7 (95th percentile) $\mu g\ m^{-3}$. This can be compared to typical background concentrations in rural areas of 1 $\mu g\ m^{-3}$.

Exposure Scenarios. The risk that a person receives depends upon a number of factors, such as

- Lifestyle (that is, did the person spend a great deal of time outdoors or doing heavy work on a farm)
- When and how long that person lived near the RFP (for example, during the key release events in 1957 and late 1960s or in the 1970s when releases were less)
- Age and gender of the person
- Where the person lived and worked in relation to the RFP.

To consider these features of a person's life, we developed profiles, or exposure scenarios, of hypothetical, but typical residents of the RFP area for which representative risk estimates could be made. Risks were calculated for nine hypothetical exposure scenarios. These scenarios incorporate typical lifestyles, ages, genders, and lengths of time in the area and can help individuals determine risk ranges for themselves by finding a lifestyle profile that most closely matches their background. The scenarios are not designed to include all conceivable lifestyles of residents who lived in this region during the time of the RFP operations. Rather, they provide a range of potential profiles of people in the area.

The nine exposure scenarios include a rancher located outside the east cattle fence along Indiana Avenue, a housewife who lived in Broomfield, a child who grows up in Broomfield during the operational period of the RFP (1953–89), and several receptors (retiree and office worker) who move into the Denver Metropolitan area in the 1970s.

Each receptor scenario incorporates inhalation rates that reflect their lifestyle. For example, the rancher's breathing rate reflects one who performs manual labor for part of the day. Uncertainty was not incorporated into the exposure scenarios; that is, the physical attributes and behavior of the receptors were assumed to be fixed. The calculated risks were not intended to represent a population of receptors who exhibit a given behavior.

Risk Estimates. Geometric mean incremental lifetime cancer incidence risk estimates for carbon tetrachloride inhalation were greatest for the rancher scenario (5.2×10^{-6}) and least for the retiree scenario (4.8×10^{-8}). The geometric standard deviations were 2.4 for both scenarios. Using the rancher scenario as an example, these risks may be interpreted as follows:

- *There is a 90% probability that incremental lifetime cancer incidence risk for the rancher was between 1.3×10^{-6} (5% value) and 2.1×10^{-5} (95% value).*
- *There is a 5% probability that incremental lifetime cancer incidence risk for the rancher was greater than 2.1×10^{-5}.*
- *There is also a 5% probability the risk was less than 1.3×10^{-6} (5% value).*

Risk estimates were within the EPA point of departure for acceptable risks (10^{-6} to 10^{-4}).

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ACRONYMS

ACGIH	American Conference of Governmental Industrial Hygienists
ASOS	Automatic Surface Observation Site
CDPHE	Colorado Department of Public Health and Environment
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
GM	geometric mean
GSD	geometric standard deviation
HAP	Health Advisory Panel
INPUFF	INtegrated PUFF dispersion code
IRIS	Integrated Risk Information System
NIOSH	National Institute for Occupational Safety and Health
OSHA	Occupational Safety and Health Administration
RAC	*Radiological Assessments Corporation*[1]
RATCHET	Regional Atmospheric Transport Code for Hanford Emission Tracking
RFP	Rocky Flats Plant
SF	slope factor
TIC	time-integrated concentration
TRAC	Terrain Responsive Atmospheric Code
USGS	U.S. Geological Survey
UTM	universal transverse mercator

[1] In 1998 *Radiological Assessments Corporation* changed its name to *Risk Assessment Corporation*. For consistency throughout the project, all reports were published by *Radiological Assessments Corporation*.

INTRODUCTION

The Rocky Flats Environmental Technology Site is owned by the U.S. Department of Energy (DOE) and is currently contractor-operated by Kaiser-Hill Company. For most of its history, the site was called the Rocky Flats Plant (RFP) and was operated by Dow Chemical Company as a nuclear weapons research, development, and production complex (Figure 1). The RFP is located on approximately 2,650 ha (6,500 acres) of Federal property, about 8–10 km from the cities of Arvada, Westminster, and Broomfield, Colorado and 26 km (16 mi) northwest of downtown Denver, Colorado. The original 156-ha (385-acre) main production area is surrounded by a 2490-ha (6150-acre) buffer zone that now delineates the RFP boundary.

This report documents risk calculations for the inhalation of carbon tetrachloride resulting from normal operational releases at the RFP from 1953–1989. A brief review of the Phase I work and carbon tetrachloride source terms is provided. This report evaluates soil and sediment monitoring data for carbon tetrachloride and discusses regulatory guidelines and evidence of carcinogenicity. It also describes environmental transport modeling, estimates of uncertainty in the model predictions, and distributions of carcinogenic risk resulting from inhalation of carbon tetrachloride for several generic receptor scenarios.

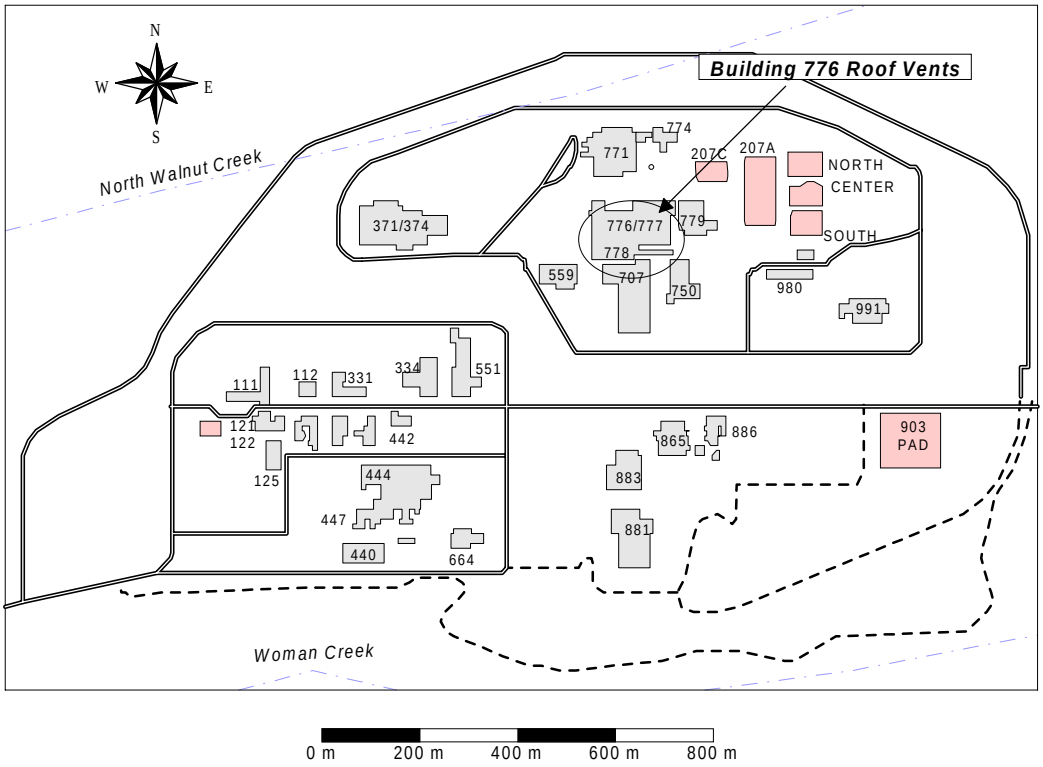

Figure 1. Main production area of the Rocky Flats Plant. Originally, the buildings were identified with two-digit numbers. Later, a third digit was added. The production area, now sometimes called the industrial area, is surrounded by a security perimeter fence. The area between the perimeter fence and Indiana Street to the east is the buffer zone. The buffer zone was expanded to Indiana Street in the 1970s. Major carbon tetrachloride release points are identified.

THE ROCKY FLATS HISTORICAL PUBLIC EXPOSURES STUDIES

Through a 1989 Agreement in Principle between the DOE and the State of Colorado, DOE provided the State with funding and technical support for health-related studies. The purpose of the Historical Public Exposures Studies on Rocky Flats is to identify potential health effects in residents in nearby communities who may have been exposed to past toxic and radioactive releases. The Colorado Department of Public Health and Environment (CDPHE) first invited a national panel of experts to help design the health studies. Because of intense public concern about Rocky Flats contamination among Denver metropolitan area residents following a Federal Bureau of Investigation raid of Rocky Flats in June 1989, the panel decided to stress public involvement and to separate the research into two major phases conducted by two different contractors to enhance accountability and credibility.

Phase I of the study was performed by ChemRisk (a division of McLaren/Hart, Environmental Engineering). In Phase I, ChemRisk conducted an extensive investigation of past operations and releases from the RFP. The Phase I effort identified the primary materials of concern, release points and events, quantities released, transport pathways, and preliminary estimates of dose and risk to offsite individuals. The conclusions from Phase I were released in a public summary document (HAP 1993), a series of task reports by ChemRisk, and several articles in the journal *Health Physics*.

Radiological Assessments Corporation (*RAC*) was awarded the contract to conduct Phase II of the study, which is an in-depth investigation of the potential doses and risks to the public from historical releases from Rocky Flats. Recommendations for work to be performed in Phase II are outlined in the Phase I summary document HAP (1993).

CARBON TETRACHLORIDE RELEASE ESTIMATES

Large quantities of carbon tetrachloride were used at Rocky Flats to clean and degrease product components and equipment. A description of how carbon tetrachloride was used and released at the RFP is provided in the Phase II carbon tetrachloride source term report (McGavran et al. 1996). Annual release estimates, release points, and the percentage contribution to the total releases from the site were reported in Phase I (ChemRisk 1992 1994a) and further verified in Phase II (McGavran et al. 1996). These estimates were based on seven inventory surveys or usage estimates, two solvent use studies, and analyses of two short-term monitoring studies. These data sources are described in Table 1 of the Phase II report (McGavran et al. 1996). The Phase I Task 5 report (ChemRisk 1994a) explains how the carbon tetrachloride source term estimates were determined and this explanation is reexamined in the source term report (McGavran et al. 1996).

The source term estimates were given in ranges for three different time periods (Table 1 and Figure 2), combining what was known about production over the years with information about efforts to phase out the use of carbon tetrachloride. The estimates are based on the conservative assumption that all of the carbon tetrachloride used evaporated into the atmosphere. This assumption was reevaluated by Rood (1997, Appendix A) who estimated the cumulative flux of carbon tetrachloride vapor to the atmosphere following a ground surface release of liquid carbon tetrachloride. A common disposal practice in the past was to dump carbon tetrachloride directly on surface soil at the RFP. Cumulative flux to the ground surface represented 90 to 95% of the

total original mass released. The remaining mass was transported to groundwater via gaseous diffusion and liquid aqueous advection. Based on these calculations, the 100% release assumption does not appear to be unreasonable.

Table 1. Carbon Tetrachloride Source Term Estimates

Time Period	Estimated release in tons per year
1953–1957	4–20
1958–1970	40–200
1971–1989	40–200 in 1970, decreasing linearly to 20–100 in 1989.

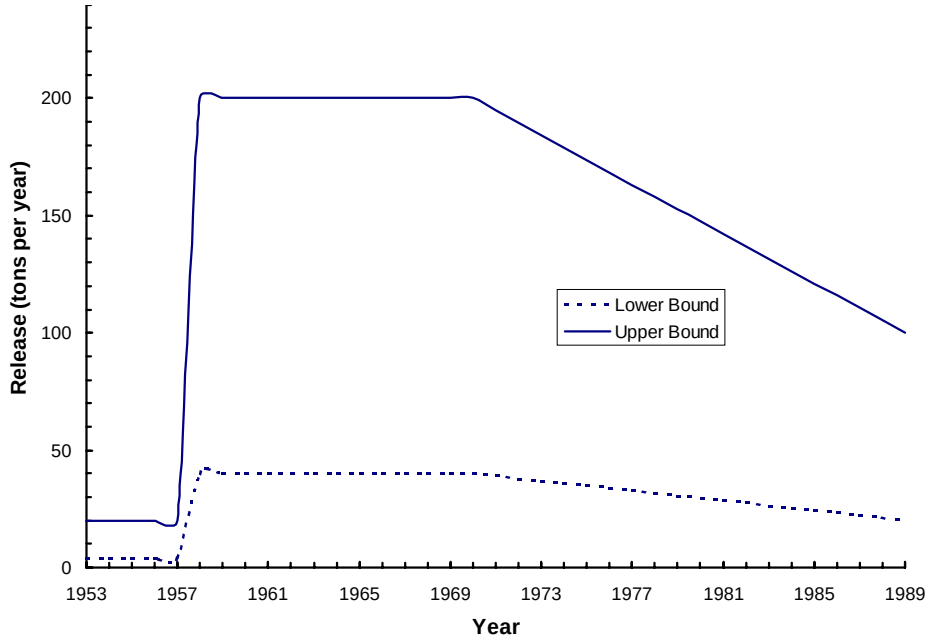

Figure 2. Carbon tetrachloride release estimates for each year of the assessment period (1953–1989).

A uniform distribution was assigned to the carbon tetrachloride source term with the minimum value equal to the lower bound estimate (0 percentile) and the maximum value equal to the upper bound (100 percentile) estimate (Figure 2).

REGULATORY GUIDELINES FOR CARBON TETRACHLORIDE

The use of carbon tetrachloride in most common household products and pesticides has been limited or banned (ATSDR 1994). Carbon tetrachloride is subject to several regulations:

- It is on the EPA's hazardous air pollutant list. Therefore the Clean Air Act requires the EPA to regulate industry sources (Hall 1997).

- It is also subject to the EPA's halogenated solvent degreasing rule (Hall 1997).
- EPA has set limits on how much carbon tetrachloride can escape from a plant into outside air. The reportable emissions quantity is currently 10 pounds (ATSDR 1994).
- The EPA has designated carbon tetrachloride as an ozone-depleting substance and has proposed its use be phased out entirely by the year 2000 (ATSDR 1994).

The Occupational Safety and Health Administration (OSHA) has set a maximum concentration limit (Permissible Exposure Limit – Time Weighted Average) in workplace air at 10 ppm (63 mg m^{-3}) for an 8 to 10 hour workday over a 40-hour work week. Before 1989, this OSHA limit was 2 ppm (12.6 mg m^{-3}). The American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value–Time Weighted Average (TLV-TWA) for carbon tetrachloride is 5 ppm (31 mg m^{-3}). The National Institute for Occupational Safety and Health (NIOSH) identifies carbon tetrachloride as a potential occupational carcinogen. The NIOSH concentration level determined as immediately dangerous to life or health (a maximum concentration above which workers must use a highly reliable breathing apparatus for protection) is 200 ppm (1,278 mg m^{-3}) (NIOSH 1994).

ENVIRONMENTAL FATE AND PATHWAYS OF INTEREST

Carbon tetrachloride is moderately soluble in water and has a low soil absorption coefficient. It is readily leached into groundwater (Howard 1991). Carbon tetrachloride contamination of groundwater at the RFP is reviewed in McGavran et al. (1996). Adsorption to sediments is not significant.

Carbon tetrachloride does not bioconcentrate (Howard 1991). Consumption of crops, fish, and other foods is probably not an important source of exposure.

Carbon tetrachloride has a relatively high vapor pressure at ambient temperatures (113.8 mm Hg at 25°C). Most of the carbon tetrachloride released to soil and surface water evaporates into the air within a few days. Carbon tetrachloride is stable in the lower layers of the atmosphere (troposphere), degrading slowly as it escapes to the higher layers. Residence times in the troposphere have been estimated to be greater than 150 years. As carbon tetrachloride diffuses into the stratosphere, it is photodegraded more rapidly. Combined, the atmospheric residence times of carbon tetrachloride in the troposphere and stratosphere range from 30 to 100 years (ATSDR 1994). Products of the photodecomposition of carbon tetrachloride can catalyze reactions that destroy ozone (ATSDR 1994). Atmospheric concentrations of carbon tetrachloride have been estimated in the northern hemisphere to range from 0.7 to 0.9 µg m^{-3} (Howard 1991). Howard (1991) also reports ambient carbon tetrachloride concentrations from 1980–82 in New Jersey to range from 0.68 to 1.5 µg m^{-3}. Atmospheric concentrations of carbon tetrachloride measured globally from 1978 to 1996 reached a peak of 0.67 µg m–3 in 1989 and have since been decreasing at an average rate of 4.5 ng m^{-3} per year (Simmonds et al. 1998.)

The inhalation pathway is clearly the exposure pathway of greatest concern for carbon tetrachloride released from the RFP. Because of the rapid volatilization of carbon tetrachloride from water and soil, the assumption that all the carbon tetrachloride inventories were released into the air is reasonable for a conservative source term estimate (see also Appendix A for an evaluation of this assumption). In addition, there was little information on releases to surface water and an absence of environmental monitoring data. For these reasons, a source term for

surface water was not developed (McGavran et al. 1996), and exposures from surface water were not determined for this assessment.

Carbon tetrachloride has been detected in the groundwater underneath the RFP but has not been detected in offsite wells and potable water supplies. McGavran et al. (1996) estimates between 1 and 15 kg of carbon tetrachloride is currently present in the aquifer underlying the RFP. This value is a relatively small fraction of the estimated annual release of the compound during the time frame of interest. The small inventory of carbon tetrachloride in the groundwater relative to the total amount used is supported by calculations presented in Appendix A.

PHASE II EXPOSURE AND RISK CALCULATIONS

Cancer Potency Determination

At their December 1994 and subsequent meetings, the Health Advisory Panel (HAP) considered the health effects of carbon tetrachloride and decided that the most appropriate endpoint for this assessment was liver cancer. Acute and chronic exposure to carbon tetrachloride can cause toxic injury to the liver, kidney, and nervous system. Carbon tetrachloride has been shown to cause liver cancer in several species and strains of experimental animals. However, case reports by physicians and studies of workers exposed to high levels of carbon tetrachloride are not conclusive. The evidence has led the U.S. Environmental Protection Agency (EPA) to classify carbon tetrachloride as a probable human carcinogen, rather than a known human carcinogen (EPA 1997).

Excess lifetime cancer incidence risk is the product of the daily carbon tetrachloride intake per unit body weight and the carcinogenic potency slope factor (SF). Slope Factors for carbon tetrachloride have been estimated by the EPA from animal studies using the linearized multistage mathematical model, which estimates the largest possible linear slope (within the 95% confidence limit) at extrapolated low doses that are consistent with the experimental data (EPA 1997). The SF is expressed in units of the inverse of milligram intake per kilogram body weight per day (kg d mg^{-1}). It represents the 95% upper confidence limit of the probability of a carcinogenic response per daily unit intake of a chemical over 70 years. The SF (and risk) is characterized as an upper-bound estimate. The true risk to humans is not likely to exceed the upper bound estimate (EPA 1995).

The unit risk value for inhalation exposure is the excess cancer risk for lifetime exposure to 1 µg of carbon tetrachloride per cubic meter of air. It is equal to the SF divided by 70 kg body weight and multiplied by the inhalation rate (20 m^3 d^{-1}) (EPA 1995).

$$UR = \frac{SF \; BR}{BW \; CF} \tag{1}$$

where

UR = unit risk (m^3 μg^{-1})
SF = slope factor (kg d mg^{-1})
BR = breathing rate (m^3 d^{-1})
CF = correction from mg to µg (1×10^3)
BW = body weight (kg).

The inhalation risk values published by the EPA in IRIS were calculated from the oral risk values assuming an air intake of 20 m^3 d^{-1} and a 40% absorption rate, based on pharmacokinetic data (EPA 1984). The EPA's Carcinogen Assessment Group determined the oral risk values using experimental animal data from four studies: hamster data from Della Porta et al. (1961) mouse data from Edwards et al. (1942): and a two National Cancer Institute studies on chloroform, 1,1,1-trichloroethane, and trichloroethylene in which carbon tetrachloride was used as a positive control (NCI 1976a, cited in EPA 1984; NCI 1976b 1977). Usually, the EPA assessment groups conservatively select data that results in the highest estimate of unit risk. Because of deficiencies in each of the studies, no one study was thought to be adequate to use alone. Therefore, all four data sets were used separately to estimate unit risk. The geometric mean of the four separate estimates is the unit risk estimate of 1.5×10^{-5} per m^3 μg^{-1} published in IRIS (EPA 1997). Using Equation 1 and the IRIS unit risk value, a SF of 5.25×10^{-2} kg d mg^{-1} is calculated. Deficiencies of the studies are discussed in detail in the *Health Assessment Document for Carbon Tetrachloride* (EPA 1984). In a discussion of confidence in IRIS (EPA 1997), the EPA states, "Since the risk estimates from these data (across 3–4 species and strains) vary by two orders of magnitude, a geometric mean of the combined data was derived as the risk estimate to accommodate the several study deficiencies."

Slope Factors calculated by EPA are designed to be protective of human health and are not intended to be true measures of the carcinogenic incidence risk to human. These SFs are typically used in risk calculations to screen contaminants, establish cleanup levels, and demonstrate no significant impacts in a prospective analysis. These endpoints are different from the endpoints of the Historical Public Exposures Studies at Rocky Flats because in this study, we are attempting to estimate the true carcinogenic risk to hypothetical individuals. For these reasons, and because preliminary risk estimates indicated carbon tetrachloride to be a major contributor to overall risk, SFs and their uncertainty were reevaluated. The distribution of SF values were calculated from the 4 animal studies used by EPA in the determination of SF values for carbon tetrachloride (Appendix B).

Uncertainties in the Slope Factors

A lognormal distribution having a GM of 2.5×10^{-2} kg d mg^{-1} and GSD of 1.4 was used to represent the distribution of the carbon tetrachloride SF in the risk calculations. Details of how this distribution was arrived at are presented in Appendix B. The SF distribution attempted to account for variation among cancer studies in rodents, metabolic conversions from animals to humans, body weight, and breathing rate variation. Other uncertainties were not quantified, but are discussed qualitatively below.

Uncertainty as to whether a threshold exists may be considerable. The cancer risk values are calculated based on an assumption of low-dose linearity, which assumes cancer can be induced at any exposure greater than zero (no threshold). A mechanism involving cell death and regeneration, leading to the development of liver tumors seems common to all of the animal studies. The EPA concluded that this damage to the liver may not be necessary to induce liver cancer and that the linear multistage model was the best way to extrapolate the risk estimates (EPA 1984).

Uncertainty also exists in extrapolating from the high dose levels used in animal studies to low doses encountered in risk assessments. Little is known about the dose-response curve at low

doses, and this extrapolation of the dose-response curve from high to low doses is a great contributor to the uncertainty. The unit risk estimate for carbon tetrachloride represents an extrapolation below the dose-response range of the experimental data. The unit risk estimates are determined using a dose-response extrapolation model that is linear at low doses.

The assumption of low-dose linearity is based on mutagenicity data and the similarities between mutagenicity and carcinogenicity. Results on the mutagenicity of carbon tetrachloride are inconclusive. This linear model may not be appropriate, so the risk values are uncertain. The EPA health assessment states, "the inconclusive nature of the presently available mutagenicity evidence for carbon tetrachloride then adds considerable uncertainty to any risk estimation based on low-dose extrapolation" (EPA 1984).

Synergistic Interactions

Alcohol consumption has been demonstrated to increase the sensitivity of people to inhalation of toxic amounts of carbon tetrachloride. Most serious and fatal cases of carbon tetrachloride poisoning have involved alcoholics or people who had several alcoholic drinks before or during their exposure (ATSDR 1992). There is some evidence that obese or undernourished people and people with gastric ulcers, diabetes, or liver disease may be sensitive to the toxic effects of ingested carbon tetrachloride (EPA 1989a). Liver toxicity may also be potentiated by exposure to other chlorinated compounds such as chlorinated solvents or pesticides. Habitual users of barbiturates may also be more sensitive (ATSDR 1992). Vitamin E, selenium and other compounds may have a protective effect against the effects of carbon tetrachloride (EPA 1984, 1989a).

How important these interactions are in increasing or decreasing the risk of cancer in people exposed to carbon tetrachloride is not known. Substances that increase the metabolism of carbon tetrachloride to toxic metabolites may also increase metabolism to carcinogenic compounds. Alcohol consumption may contribute to liver cancer, and it is reasonable to theorize that people that consume alcohol may be at greater risk of developing liver cancer from carbon tetrachloride exposure. People who consume relatively large amounts of alcohol may be among the more sensitive people in the general population.

Current risk assessment methodology uses this information qualitatively (EPA 1984). Whether interactions found in the laboratory are important for people exposed to contaminants in the environment is not known. The probabilities of synergistic and antagonistic reactions occurring in the general population are not available.

ENVIRONMENTAL TRANSPORT MODELING

Offsite exposure to carbon tetrachloride originating from RFP was investigated in Phases I and II (McGavran et al. 1996) and summarized in the previous sections. Airborne releases were considered to be the major pathway of exposure. Surface water releases of carbon tetrachloride were expected to volatilize and become part of the atmospheric source term. For these reasons, only atmospheric transport of carbon tetrachloride was considered.

We have assumed most of the carbon tetrachloride routinely used at the RFP evaporated during cleaning and degreasing operations and was vented to the atmospheric via roof vents on Buildings 776 and 707 where operations of this type were performed. Leftover carbon

tetrachloride was believed to be dumped in burn pits and on the soil. Small amounts of carbon tetrachloride were also released from numerous other release points identified in the Phase I reports. In this section, we describe our approach to estimating atmospheric dispersion of carbon tetrachloride for the years 1953–1989 and the uncertainty associated with concentration estimates in the model domain. Our approach to this calculation involves first estimating an annual average X/Q (concentration divided by source term [s m^{-3}]) for each receptor in the model domain. Concentrations for specific years of the assessment period are calculated by multiplying the annual quantity of carbon tetrachloride released to the atmosphere by the X/Q value for a given receptor located in the model domain. Uncertainties in dispersion estimates are accounted for through multiplicative correction factors. Airborne concentrations are then used with exposure scenarios and the SFs to calculate risk for selected receptors in the model domain.

Atmospheric Model Selection

Five atmospheric transport models considered for use in this study were evaluated in Rood (1997): (1) the Terrain-Responsive Atmospheric Code (TRAC) (Hodgin 1991), (2) the Industrial Source Complex Short Term Version 2 (ISC) (EPA 1992), (3) Regional Atmospheric Transport Code for Hanford Emission Tracking (RATCHET) (Ramsdell et al. 1994), (4) TRIAD (Hicks et al. 1989), (5) and INPUFF2 (Petersen and Lavdas 1986). The purpose of the model comparison study was to determine what models, if any, performed best in the Rocky Flats environs for a given set of modeling objectives. These data along with other studies were used to establish the uncertainty one might expect from a model prediction.

Model evaluations were based on how well predictions compared with measured tracer concentrations taken during the Winter Validation Tracer Study (Brown 1991) conducted in February 1991 at the RFP. The study consisted of 12 separate tests; 6 tests were conducted during nighttime hours, 4 during daytime hours, and 2 during day-night transition hours. For each test, an inert tracer (sulfur hexafluoride) was released in an open area near the southern RFP boundary. The tracer was released at a constant rate for 11 hours from a 10 m high stack. Two sampling arcs, 8 and 16 km from the release point, measured tracer concentrations every hour for the last 9 hours of each test period. Seventy-two samplers were located on the 8-km arc, and 68 samplers were located on the 16-km arc. Predicted concentrations were then compared to the observed tracer concentrations at each of the samplers.

Modeling objectives for the comparison study were based on the premise that identifying locations of individual receptors on an hour-by-hour basis was unlikely. Instead, it was more likely to identify receptors (hypothetical or real) who were present at a fixed location for the duration of a release event. The minimum time scale of historical release events at RFP ranged from one to several days. Release events modeled for the Winter Validation Tracer Study were 9 hours in duration. If we assume the receptor is fixed for a time period of at least 9 hours, then the time-averaged concentration (9-hour average) is an appropriate modeling objective rather that comparing hourly average concentrations. Therefore, models were evaluated based on their performance in predicting time-averaged concentrations at fixed sampler locations in the model domain (9-hour average concentration at each sampler paired with the corresponding predicted value). We also considered the arc-integrated concentration. The arc-integrated concentration was the 9-hour average ground-level concentration integrated across the 8 and 16-km sampling arc. The latter performance objective provides a measure of the vertical dispersion component of

the models and the ground-level tracer mass, 8 and 16-km from the release point. Data sets for the time-averaged concentration were limited to only those points where the predicted (C_p) and observed (C_o) concentration pair were greater than the time-averaged minimum detectable concentration.

Fifty percent of the time-averaged model predictions were within a factor of 4 of the observations. Predicted-to-observed ratios (C_p/C_o) ranged from 0.001 to 100 and tended to be higher at the 16-km arc than the 8-km arc. Geometric mean C_p/C_o ratios ranged from 0.64 (TRAC) to 1.5 (ISC), and geometric standard deviations ranged 4.4 (RATCHET) to 6.5 (ISC). The RATCHET model had the highest correlation coefficient for the 8-km (0.67) and 16-km (0.58) sampling arc followed by TRIAD and INPUFF2.

Arc-integrated results (Figure 3) showed INPUFF and TRIAD had the highest correlation coefficients, but correlation coefficients were not significantly different (at the 95% level) from the other models. Qualitatively, the predictions made by the RATCHET model appear to best match the observations. The slope of the regression line was closest to that of the perfect correlation line (solid line in Figure 3). The ISC model tended to overpredict arc-integrated concentration, and the TRAC model showed the greatest variability.

The results reported in Rood (1997) indicated no one model clearly outperformed the others. However, the RATCHET, TRIAD, and INPUFF2 models generally had lower variability (indicated by lower geometric standard deviations of C_p/C_o ratios) and higher correlation coefficients compared to those of ISC and TRAC models. It is desirable in a study such as this to choose a model that has the least amount of variability when comparing model predictions to observations. In addition, the model selected should have a level of complexity that is consistent with available data. The TRAC model is the most complex in terms of its treatment of the atmospheric dispersion process in complex terrain, but the study showed model performance was no better than the other models. In addition, the availability of meteorological data needed to fully use the capabilities of the TRAC model are lacking. The straight-line Gaussian plume model, ISC, tended to overpredict concentrations and was also limited to only one meteorological recording station in the model domain. Available meteorological data for this study period may include two meteorological recording stations: one at the RFP and the other at Denver Stapleton International Airport. Therefore, a model that may include multiple meteorological recording stations in the model domain is desirable. The use of multiple meteorological recording stations will allow for a spatially varying wind field in the model domain.

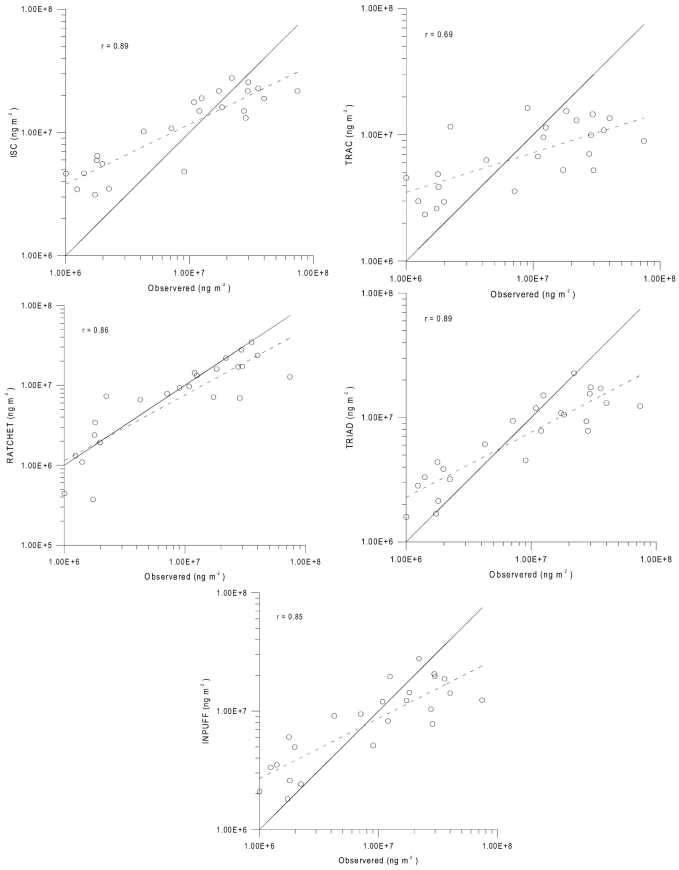

Figure 3. Observed arc-integrated concentration as a function of predicted values for the five models compared using the Winter Validation Data Set. Correlation coefficients were for the log-transformed data. The solid line represents perfect correlation between predicted and observed values. The dashed line represents the log-transformed regression fit.

The three models RATCHET, INPUFF2, and TRIAD performed comparably and were considered viable candidates for atmospheric dispersion estimates. We chose the RATCHET model for modeling routine releases of carbon tetrachloride for the following reasons:

- The model is easily configured for long-term (annual average) dispersion estimates
- Spatial differences within the model domain are accounted for (i.e., surface roughness meteorology)
- Algorithms to compute plume depletion and dry and wet deposition for gases are included (deposition must be computed outside the TRIAD and INPUFF2 codes)
- The model requires meteorological data in 1-hour increments, which are the same as those given for typical airport observations.

Corrections for model bias were made in the uncertainty analysis. Table 2 summarizes features of the RATCHET model.

Table 2. Features of the RATCHET Model

Feature	Representation in RATCHET
Domain area[a]	2100 km^2
Node spacing[a]	2000 m
Source term	Hourly release rates
Meteorological data	Hourly
Surface roughness	Spatially varying
Wind fields	1/r^2 interpolation
Topographical effects	None explicit[b]
Wind profile	Diabatic
Stability	Spatially varying based on wind, cloud cover, and time of day
Precipitation	Spatially varying, three precipitation regimes with different precipitation rate distributions
Mixing layer	Spatially varying, based on calculated values for each meteorological station
Plume rise	Briggs' equation (Briggs 1969, 1975, 1984)
Diffusion coefficients	Based on travel time and turbulence levels
Dry deposition	Calculated using resistance model
Wet deposition	Reversible scavenging of gases, irreversible washout of particles
Model time step	15 minute maximum, 15 second minimum
Output frequency[c]	Daily
Uncertainty	Options available for Monte Carlo simulation within the code

[a] Modified from the original RATCHET specification for use at Rocky Flats

[b] The model does not account for terrain elevation changes relative to the plume height explicitly. However, topographical influence on the wind field may be accounted for by incorporating multiple meteorological stations in the model domain.

[c] Modified to output annual average concentrations at user specified grid nodes

Model Domain and Receptor Grid

The model domain (Figure 4) encompasses a 2,200 km^2 area (50 km north-south by 44 km east-west). The domain extends 28 km south, 12 km west, 22 km north, and 32 km east from the RFP. Most of the Denver metropolitan area and the city of Boulder were included in the domain. The domain was limited in its western extent because few receptors are present there and most of the contaminant plumes traveled east and southeast of the RFP.

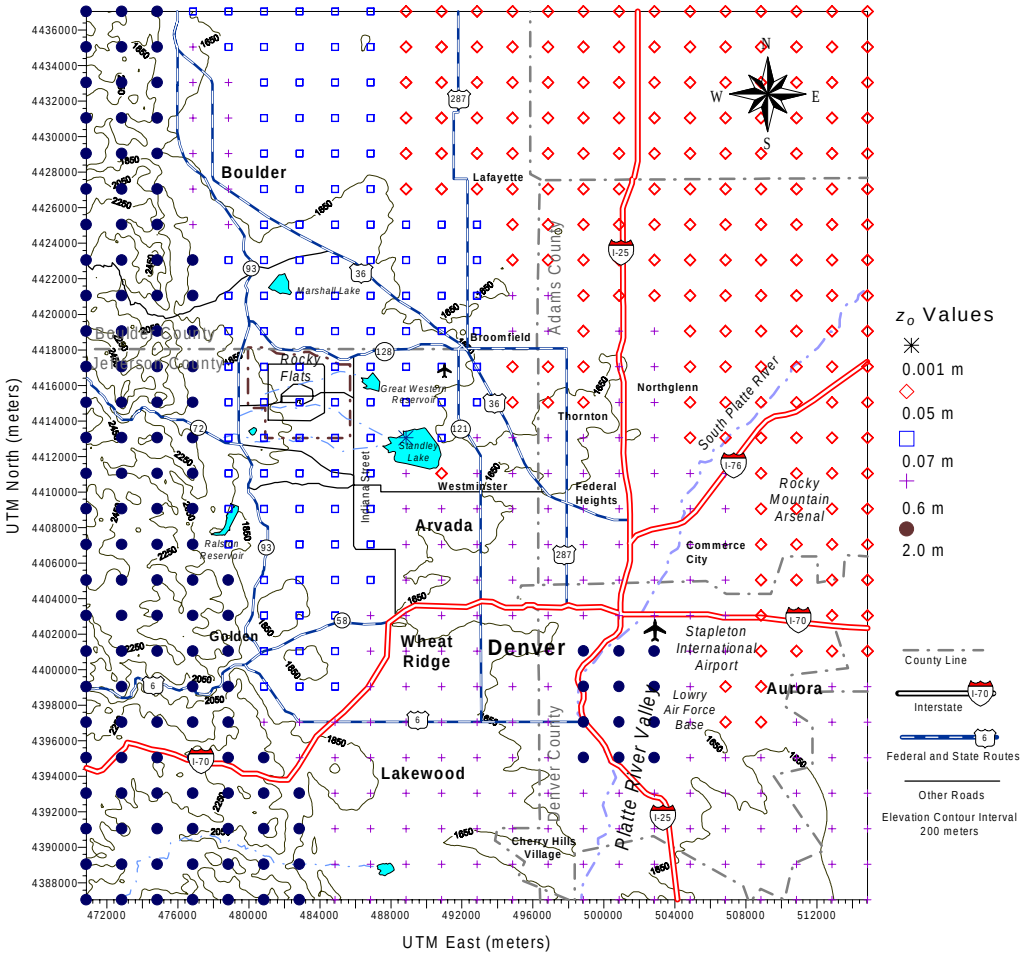

Figure 4. RATCHET environmental modeling grid and roughness length values (z_o). Symbols represent grid nodes and the z_o value assigned to the node.

RATCHET uses two modeling grids. Hourly meteorological records are used to estimate wind speed and direction, stability, and precipitation on the environmental grid in addition to surface roughness features. The concentration grid has spacing one-half that of the environmental grid. Ground-level concentrations and deposition are output at each of these grid nodes. The environmental grid was set at 23 nodes east-west and 26 nodes north-south with a grid spacing of 2000 m. The concentration grid has 45 nodes east-west and 51 nodes north-south with a spacing of 1000 m. The southwest corner of the model domain has the Universal Transverse Mercator (UTM) coordinates 470850 E and 4387050 N. Release points are defined by distances (in kilometers) from a reference node. The reference node for the environmental grid was 7,15 and 13,29 for the concentration grid. Both have the UTM coordinates of 482850 E and 4415050 N.

Figure 4 was generated using United States Geological Survey (USGS) 7.5-minute digital elevation models. Topographic contours were based on an elevation grid spacing of 100 m. Major roadways were digitized from United States Geological Survey (USGS) 1:100,000 digital line graphs.

Meteorology

Meteorological data for the operational period of Rocky Flats (1952–1988) are sporadic, incomplete, and of questionable integrity. Requests for meteorological data from the RFP were initially made by ChemRisk during Phase I of the project. ChemRisk was able to locate two letters from Dow Chemical to Dr. Roy Cleare, Executive Director of the Colorado Department of Health, dated March 20, 1970, that contained wind speed and direction for varying time increments during the 1957 and 1969 fire incidents. Computer diskettes containing wind speed, wind direction, and precipitation measurements from October 1968 to May 1969 were also obtained. These data were hourly observations taken approximately 15 minutes before the top of the hour and do not represent hourly average readings. Although these data appeared to be climatologically reasonable, no records of instrument calibration or audits of the information were found. Parameter resolution was very coarse (for example, wind direction resolution was 45 degrees). Five years (1987–1991) of high quality meteorological data taken at the 61-m tower at RFP were obtained and used by ChemRisk in Phase I of this project for predicting annual average concentrations from routine releases.

An extensive data search was initiated in 1994 by *Radiological Assessments Corporation (RAC)* researchers to locate missing data and interview personnel who were involved with measurements at the site. No new data were recovered, but several personnel reported problems with the recording instrumentation at the RFP, such as the measured wind direction being off by 180 degrees. Other data recorded from nearby Jefferson County Airport (about 8 km east of the RFP) were obtained for the years 1968–1971. These data were only reported for the hours while the airport was open (06:00–23:00 local standard time) and were instantaneous measurements and not hourly averages as was typical of all airport data before the Automatic Surface Observation Site (ASOS) system was installed at most major airports. In 1994, the RFP hired a subcontractor to compile, screen, validate, and analyze historical climatological data (DOE 1995). A draft report was issued in February 1995; the report contained monthly and annual summaries of wind speeds, wind directions, precipitation, temperature, and other parameters for the years 1953–1993. While these data are of interest and may be important for some aspects of modeling, they lacked the resolution required for detailed atmospheric transport modeling.

We concluded that meteorological data taken during the time the RFP was operating were incomplete, unreliable, and unsuitable for atmospheric transport modeling during the period, 1953–1989. However, surrogate data spanning a different time period can be used to make annual average dispersion estimates for past releases. We used this approach in our modeling effort.

For our modeling effort, we used meteorological data spanning a 5-year period (1989–1993) taken at two recording stations located at the RFP and Denver Stapleton International Airport. Federal regulations have stated that a 5-year database is adequate for predicting annual-average air quality impacts at a site (CFR 1996). Meteorological data from RFP were taken at the 10-m level from the 61-m tower located on the south side of the plant complex at UTM coordinates 482064 E 4414963 N. Data recorded at this station included wind speed, wind direction, temperature, and other parameters (heat flux, and standard deviation of wind direction) that were not used in these simulations. The Denver Stapleton meteorological station was located 24 km east and 14 km south from the center of the model domain (RFP). These data included hourly measurements of wind speed, wind direction, cloud cover, and precipitation. It is known that

meteorological conditions in the Denver metropolitan area can differ significantly from those at Rocky Flats (DOE 1980). Therefore, it is unreasonable to use meteorological data from Denver alone for simulations involving releases from Rocky Flats. In these simulations, initial plume trajectories are primarily influenced by the wind direction at Rocky Flats. Only after plume elements are transported to the Denver metropolitan area are trajectories and dispersion influenced by meteorological conditions present there.

Data Processing

Meteorological data from 1989–1993 were obtained in electronic format from the Rocky Flats meteorologist. These data were measured at a height of 10 and 61 m from a 61-m tower located at RFP. Only data from the 10-m level were used in the simulations. Each record represented the average over a 15-minute recording period and included wind speed and direction, temperature, heat flux, and standard deviations of these parameters. Processed data suitable for use in EPA's ISC code were also obtained for the same time frame. These data included stability class estimated by the lateral turbulence and wind speed method (standard deviation of the horizontal wind direction fluctuations) as described in EPA (1987) and mixing height estimates. The mixing heights were derived from linear interpolation for each 15-minute period from the rawinsonde data furnished routinely every 12 hours by the National Weather Service for Denver Stapleton International Airport. These data were used as default mixing-layer depths in RATCHET. Mixing-layer depths are calculated hourly within RATCHET at each active meteorological recording station using a methodology described by Zilitinkevich (1972). The calculated or default value is selected on the basis of the relative magnitude of the calculated and default values, the stability, season, and time of day. The larger of the two is selected for the meteorological recording station for the given hour. A multiple linear regression technique is then used to provide a smooth spatial variation in mixing-layer depth across the model domain.

Stability classes were calculated separately for the RFP and Denver Stapleton International Airport meteorological recording stations using the general classification scheme discussed in Pasquill (1961), Gifford (1961), and Turner (1964). This typing scheme employs seven stability categories ranging from A (extremely unstable) to G (extremely stable) and requires estimates of sky cover and ceiling height. Cloud cover and ceiling height data for both stations were assumed to be the same and were obtained from the Denver Stapleton International Airport data.

Hourly average wind speed and direction also were calculated from the raw RFP meteorological data using the protocol described in EPA (1987). An arithmetic average of the wind direction was computed first, and it was then segregated into 1 of 36, 10-degree increments as required by RATCHET. The average wind speed for the hour was computed by taking the average of the four, 15-minute data segments. Hourly precipitation records from Denver Stapleton International Airport were assumed to be consistent over the entire model domain and were segregated into integer values as required by RATCHET (see Table 4).

Atmospheric Transport Model Parameters

This section describes the input parameters that were selected for the RATCHET model for simulations involving normal operational releases. These parameters include surface roughness length, topography, dry and wet deposition, diffusion coefficients, release parameters (location

and height of release), and model control parameters (number of puffs per hour and computational options).

Surface Roughness Length

Roughness elements such as trees and buildings and small-scale topographic features (such as rolling hills) have a frictional effect on the wind speed nearest the surface. The height and spacing of these elements will determine the frictional effects on the wind. These effects are directly related to transport and diffusion and affect atmospheric stability, wind profiles, diffusion coefficients, and the mixing-layer depth. The surface roughness length parameter is used to describe these roughness elements and is a characteristic length associated with surface roughness elements (Table 3). In RATCHET, estimates of the surface roughness length are defined for each node on the environmental grid (Figure 4). In our simulations, we selected a value of 0.6 m to represent residential and urban environs. Farmland, which is predominant in the northeast part of the model domain, was assigned a value of 0.05 m. Range and open land consisting of rolling grass hills were assigned a value of 0.07 m. Nodes that encompass the range and farmland designation were selected based on the topographic contours and land use maps. The foothills and downtown Denver were assigned a value of 2.0 m and open water (Standley Lake) was assigned a value of 0.001 m.

Table 3. Typical Surface Roughness Lengths for Different Land Use, Vegetation, and Topographic Characteristics

Land use, vegetation, and topographic characteristics	Surface roughness length, z_o (m)
Level grass plain	0.007–0.02
Farmland	0.02–0.1
Uncut grass, airport runways	0.02
Many trees/hedges, a few buildings	0.1–0.5
Average, North America	0.15
Average, U. S. Plains	0.5
Dense forest	0.3–0.6
Small towns/cities	0.6–2.5
Very hilly/mountainous regions	1.5+
[a] Source: Stull (1988) Figure 9.6.	1.5+

Topography

The RATCHET model does not explicitly address terrain differences within the model domain. Instead, topography and topographic effects on transport and diffusion are reflected in the surface roughness lengths and observed wind velocity data that are affected by topographical features. Topography in the model domain (Figure 4) can be characterized by three major features: the north-south trending Colorado front range foothills in the western part of the model domain, the southwest to northeast trending Platte River Valley located in the southeast part of the model domain, and rolling hills and flat farmland that is predominant in the central and northeastern part of the model domain. The surface roughness lengths reflect these features as stated in the previous section. Observed meteorological data are lacking in most of the model domain and are woefully inadequate to characterize wind fields in the foothills region. However,

meteorological observations at Denver Stapleton International Airport do capture the air movement within the Platte River Valley, which is noticeably different than that at the RFP (DOE 1980). Therefore, to a limited extent, topography is accounted in the model simulation. The use of a complex terrain model would also suffer from the lack of meteorological data, especially in the foothills region. This region may be of little importance because few receptors were present in the foothills when the plant was operating.

Dry and Wet Deposition

Carbon tetrachloride was assumed to exist as a gas in the environment and was modeled as such. The compound is generally thought to be very stable in the troposphere with residence times between 30 and 50 years. Its main loss mechanism is diffusion to the stratosphere where it photolyzes. Less than 1% of the carbon tetrachloride released to the atmosphere is partitioned into large water bodies (Howard 1991). For these reasons, carbon tetrachloride was modeled in RATCHET as a slightly reactive gas. The dry deposition properties of a slightly reactive gas are similar to those of small particles. The rate of deposition of small particles and gases on surfaces in the absence of precipitation is proportional to the concentration of material near the surface. The proportionality constant between the concentration in air and the flux to the ground surface is the dry deposition velocity. The current generation of applied models estimates deposition using an analogy with electrical systems as described by Seinfeld (1986). The deposition is assumed to be controlled by a network of resistances, and the deposition velocity is the inverse of the total resistance. Resistances are associated with atmospheric conditions; physical characteristics of the material; and the physical, chemical, and biological properties of the surface. The total resistance in RATCHET is made up of three components: aerodynamic resistance, surface-layer resistance, and transfer resistance. Thus, the dry deposition velocity (v_d, m s^{-1}) is calculated using

$$v_d = (r_s + r_a + r_t)^{-1} \quad (2)$$

where

r_s = surface layer resistance (s m^{-1})
r_a = aerodynamic resistance (s m^{-1})
r_t = transfer resistance (s m^{-1}).

Surface layer resistance and aerodynamic resistance are given by

$$r_a = U(z)/u_*^2 \quad (3)$$

$$r_s = 2.6/(0.4\, u_*) \quad (4)$$

respectively where u_* = frictional velocity (m s^{-1}), and $U(z)$ = wind speed (m s^{-1}) measured at height z (m) above the ground. The frictional velocity is given by

$$u_* = \frac{U(z)\,k}{\ln\left(z / z_o\right) - \psi(z / L)} \quad (5)$$

where k = the von Karman constant (0.4), z_o = surface roughness length, ψ = stability correction factor, and L = the Monin-Obukhov length (m). The transfer resistance is associated with the characteristics of the depositing material and surface type. In RATCHET, the transfer resistance is used as a mathematical means to place a lower limit on the total resistance. As the windspeed increases, r_s and r_a become small resulting in unreasonably high deposition velocities. For small

particles (<1.0 μm) and slightly reactive gases, a transfer resistance of 100 s m^{-1} is suggested in RATCHET, and it results in calculated deposition velocities that are consistent with measured data. Harper et al. (1995) estimates deposition velocities for 1 μm particles and 5 m s^{-1} wind speed to range from 1.0×10^{-2} (5th percentile) to 4.1 cm s^{-1} (95th percentile). The RATCHET calculated values assuming a roughness length of 0.05 m and a transfer resistance of 100 s m^{-1} ranged from 0.66 to 0.75 cm s^{-1}, which is in the range of measured values.

Table 4. Precipitation Rates and Precipitation Codes Used in RATCHET

Precipitation type	Precipitation rate (mm hr^{-1})	RATCHET precipitation code
No precipitation	0.0	0
Light rain	0.1	1
Moderate rain	3.0	2
Heavy rain	5.0	3
Light snow	0.03	4
Moderate snow	1.5	5
Heavy snow	3.3	6

Wet deposition of gases in RATCHET is modeled using a wet deposition velocity (Slinn 1984) and assuming equilibrium between the gas concentration in air and precipitation. Slinn (1984) gives the following expression for estimating the wet deposition velocity for gases:

$$d_{vw} = C\ S\ P_r \tag{6}$$

where

d_{vw} = wet deposition velocity (m s^{-1})
C = a conversion factor from mm hr^{-1} to m s^{-1}
S = solubility coefficient
P_r = precipitation rate (mm hr^{-1}).

The solubility coefficient is inversely related to the Henry's Law constant and is given by

$$S = \frac{R\,T}{H} \tag{7}$$

where R = the universal gas constant (8.23×10^{-5} m^3 atm mol^{-1} K^{-1}), T = temperature (Kelvin), and H = Henry's Law constant for carbon tetrachloride (3.04×10^{-2} atm m^3 mol^{-1} at 24.8° C). Precipitation rates in RATCHET are separated into six classes: three for liquid and three for frozen precipitation. Each class is assigned a precipitation code (0 for no precipitation). The RATCHET default precipitation rates were assigned to each class as given in Table 4. These classes are similar to those reported by most airport meteorological recording stations. Scavenging of reactive and nonreactive gases by snow when the temperature is less than –3°C is low. RATCHET ignores wet deposition under these conditions.

Diffusion Coefficients

The RATCHET model estimates the diffusion coefficients directly from statistics for atmospheric turbulence. In most cases, the statistics describing atmospheric turbulence (i.e., standard deviation of the horizontal and vertical wind direction fluctuations) are not routinely

measured at most meteorological recording stations. However, RATCHET makes use of atmospheric conditions that are either measured or calculated from routine meteorological data to estimate the turbulence statistics. The parameters wind speed, atmospheric stability, and surface roughness are used to estimate the turbulence statistics. The general form of the equation used in RATCHET for estimating the horizontal diffusion coefficient (σ_r), for the first hour following release is

$$\sigma_r = 0.5\sigma_v\, t \tag{8}$$

where σ_v = crosswind component of turbulence (m s^{-1}) and t is the travel time. After the first hour, the horizontal diffusion coefficient is given by $\sigma_r = c_{sy}$ t where c_{sy} is a proportionality constant with dimensions of meters per second. Gifford (1983) has shown the value of c_{sy} distributed between 0.14 to 1.4 with a median value of 0.5. For our simulations, we used the median value of 0.5.

The general form of the equation for estimating the vertical diffusion coefficient (σ_z) near the source is

$$\sigma_z = \sigma_w\, t\, f_z(t) \tag{9}$$

where

σ_w = standard deviation of the vertical component of the wind (m s^{-1})

$f_z(t)$ = nondimensional function related to the travel time and turbulence time scale.

As a practical matter, diffusion coefficients in RATCHET are calculated in increments to avoid problems associated with spatial and temporal changes in conditions.

Source Characterization

Estimated releases of carbon tetrachloride to the atmosphere were extracted from ChemRisk (1994a) and summarized in McGavran et al. (1996). Eighty percent of the emissions were attributed Building 707 and 20% were attributed to Buildings 776 and 777 (ChemRisk 1992). However, total release estimates were not consistent with this partitioning of releases between buildings because the largest releases occurred before construction of Building 707 was completed in 1972. (The 80% value may have referred to controlled releases and pre-1972 releases may have been considered uncontrolled). Building 707 emissions originated from two inverted "J" roof vents similar to those used in Buildings 776 and 777 (vents #9/10 and #36 accounted for 99% of the Building 707 releases, ChemRisk [1992] page B-47). For modeling purposes, all emissions were assumed to originate from Buildings 776 and 777. This simplification was made because of the similar release conditions for both buildings and the close proximity of Building 707 to Buildings 776 and 777. Similar release heights and location result in similar *X/Q* values calculated at receptors of interest for both buildings.

Releases from Building 776 were reported to originate from five, "J" shaped roof vents. The vents directed flow down toward the top of the roof. Therefore, the modeled release height was the height of the building. The building height was 11.6 m and the horizontal dimensions were 61 m × 104 m. Effluent temperature was assumed to be 20 degrees C, the typical temperature of the ambient air in the building. The vents were assumed to be distributed across the roof resulting in an area source geometry. The area source was simulated by modifying the initial diffusion coefficients using a procedure described by Petersen and Lavdas (1986). The initial horizontal diffusion coefficient (σ_r) is the horizontal dimension of the source divided by 4.3, and the initial

vertical diffusion coefficient (σ_v) is the height of the source divided by 2.15. For these simulations, we used the 61-m length as the horizontal source dimension (Table 5).

Table 5. Release Parameters for Building 776

Release point	Parameter	Value
Building 776 roof vents	Release height	11.6 m
	Initial σ_r	14.1 m
	Initial σ_v	5.4 m
	UTM east	482938 m
	UTM north	4415879 m

Stack tip downwash is also modeled in RATCHET; however building wake is ignored. Building wake affects only those receptors relatively close to the source. At distances of about 2 km, building wake has been shown to have little effect on measured atmospheric concentrations (Start et al. 1980). Ramsdell (1990) showed that for ground-level releases, modeled air concentrations greater than 1 km from the source are relatively unaffected by building wakes. Note the nearest receptor is >3 km from building 776.

Release estimates (Table 1 and Figure 2) were reported as a range of possible values. For the uncertainty analysis, the source term was assigned a uniform distribution having a minimum and maximum value that corresponded to the upper and lower bound estimate.

Other Parameters

Several other parameters in RATCHET influence the accuracy of output and computer runtime. These parameters include the number of puffs per hour, minimum time step, puff consolidation, maximum puff radius, and minimum puff concentration at center. We chose the suggested RATCHET default values for all these parameters except minimum time step and minimum concentration at puff centers (Table 6). Accuracy of the simulation can be improved by using a smaller time step. The RATCHET default was 20 minutes, which we reduced to 10 minutes. The minimum concentration at puff centers was reduced from 1×10^{-13} to 1×10^{-15} to allow for plume tracking throughout the model domain. The puff consolidation parameter value combines puffs from the same source when ratio of the puff centers to the average σ_r is less than the user-input value. The puff consolidation ratio and maximum puff radius (in units of σ_r) were set at RATCHET default values of 1.5 and 3.72, respectively.

Table 6. RATCHET Model Control Parameters

Model parameter	Value
Number of puffs per hour	4
Minimum time step	10 minutes
Puff consolidation	1.5
Maximum puff radius (in units of σ_r)	3.72
Minimum concentration at puff centers	1×10^{-15}

Prediction Uncertainty

We are interested in defining the expected uncertainty in the annual average dispersion estimates within the model domain for each year of the assessment period (1953–1989). The approach used in this assessment to define uncertainty in predicted concentrations was to develop distributions of multiplicative correction factors that were applied to each deterministic concentration in the model domain. These multiplicative correction factors were developed from field validation data, joint frequency distribution comparisons, and parametric uncertainty analysis. Three components of uncertainty were evaluated:

1. Dispersion uncertainty
2. Meteorology uncertainty
3. Plume depletion uncertainty.

Dispersion uncertainty considers the uncertainty in predicting the annual average concentration of an inert, non-reactive tracer for a specific year, assuming we have the meteorological data for that year. Meteorology uncertainty arises because we are using 5 years of meteorological data spanning a recent time period (1989–1993) to calculate an annual average *X/Q* value (concentration divided by release rate) that will be applied to all previous years (1953–1989) of the assessment period. Uncertainty in plume depletion via dry deposition was considered separately because dispersion uncertainty was based on tracer studies that typically employ inert, non-reactive tracers that have dry deposition velocities that are small and inconsequential. Uncertainty in plume depletion from wet deposition was not considered.

Dispersion Uncertainty. Dispersion uncertainty includes two sources; 1) errors in model input and, 2) errors in model formulation or in the model itself (i.e., does the model adequately represent the physical process and phenomena it attempts to simulate). For example, suppose we select a location in the model domain and measure the concentration of tracer released from the site for an entire year. Let us assume the uncertainty associated with the measurement is small and inconsequential. Using the meteorological data recorded for that year, we calculate a concentration at the same receptor location using an appropriate atmospheric dispersion model. Assuming our model adequately represents the physical process and phenomena (i.e., if we had the correct inputs to the model, the output would match the observations), the uncertainty associated with the model prediction results from a lack of knowledge about the correct inputs to our model. Propagating these uncertainties through the model calculation provides a distribution of model output. This is termed parameter uncertainty. The output distribution may be compared with measured data to see if model predictions encompass the measurements. Generally, agreement between predictions and observations is achieved when the model adequately represents the processes it attempts to simulate and choices regarding input parameter values have been made correctly.

Model uncertainty arises from the fact that perfect models cannot be constructed, and models often fail to adequately represent the physical process they attempt to simulate. In atmospheric dispersion models, the advection-dispersion process is often oversimplified and meteorological data required to characterize turbulence in the environment are lacking. In our previous example, the parameter uncertainty may not account for all differences between model predictions with observations if our model does not perfectly represent the physical process. Field validation exercises provide some information as to the overall performance of a model and, in turn, model

uncertainty. However, these are only partially relevant because field tests are generally not conducted under the same conditions that actual releases occurred.

The RATCHET model incorporates modules to explicitly assess parameter uncertainty. These parameters include wind direction, wind speed, atmospheric stability class, Monin-Obukhov length, precipitation rate, and mixing-layer depths. Other parameters may be assessed by simply varying the input according to some predefined distribution and repeating the simulation a number of times until an adequate output distribution is achieved. These methods are both time consuming and computationally intensive and fail to capture model uncertainty. In our approach, we ignored the built-in parameter uncertainty in RATCHET and focused our efforts on defining the distribution of a correction factor that will be applied to model output. (Parameter uncertainty was only used to evaluate uncertainty in plume depletion and deposition.) The correction factor was based on field experiments, considering the relevance of the experiment to actual release conditions and model domain environs. In this approach, we have ignored the mass balance features of RATCHET and have instead, treated model output like that of a straight-line Gaussian Plume model. The only difference being that plume trajectories are not limited to straight lines.

We begin the process of defining the distribution of the correction factor for dispersion uncertainty by reviewing some field studies considered relevant to the assessment question (Table 7) which is what is the annual average concentration for each year of the assessment period. The correction factor is defined as the inverse of the distribution of predicted-to-observed ratios $[1/(C_p/C_o)]$. Relevant field studies included a model evaluation using the Rocky Flats Winter Validation Tracer Study data set (Rood 1997), validation exercises for RATCHET performed at the Hanford Reservation (Ramsdell et al. 1994), summaries of model validations performed for the Gaussian plume model (Miller and Hively 1987), and other studies reported in the literature. No one study is entirely relevant. Averaging times, release conditions, meteorological conditions, and terrain conditions are different than what we are attempting to simulate in this study. Nevertheless, these are the data we have chosen to work with and it is unlikely we will find a field validation experiment that was conducted under the exact conditions of past releases at Rocky Flats. Uncertainty bounds may be expanded to compensate for our lack of knowledge.

Table 7. Geometric Mean and Geometric Standard Deviation of Predicted-to-Observed Ratios for Field Studies Relevant to Defining the Correction Factor for Annual Average Concentrations

Model	Averaging time	Receptor distance	Release height	Environment	GM	GSD	Comments
RATCHET[a]	9-hour	8 km	10 m	Complex terrain	0.86	4.4	Rocky Flats Winter Validation Study
RATCHET[a]	9-hour	16 km	10 m	Complex terrain	1.1	4.3	Rocky Flats Winter Validation Study
RATCHET[b]	28-day	20–80 km	61 m	Flat	1.4	2.2	Conducted at the Hanford Reservation
Gaussian Plume[c]	Short-term	10 km	ground level	Flat - highly instrumented		1.1	Predicted/observed (P/O) ratios ranged from 0.8 to 1.2
Gaussian Plume[c]	Short-term	10 km	elevated	Flat - highly instrumented		1.2	P/O ratios ranged from 0.65 to 1.4
Gaussian Plume[c]	Short -term	—	—	Complex terrain		14	P/O ratios ranged from 0.01 to 100
Gaussian Plume[c]	Annual average	—	—	Complex terrain		3.8	P/O ratios ranged from 0.1 to 10
Gaussian Plume[c]	Annual average	10 km	ground-level	Flat		1.5	P/O ratios ranged from 0.5 to 2
Gaussian Plume[c]	Annual average	10–150 km	ground-level	Flat		2.2	P/O ratios ranged from 0.25 to 4
Gaussian Plume[d]	12-hour	1–5 km	60 m	Relatively flat	0.82	3.4	Terrain heights varied by about 50 m
Gaussian Plume[d]	72-hour	1–5 km	60 m	Relatively flat	0.67	2.1	Terrain heights varied by about 50 m
Eulerian and Gaussian Plume[e]	Annual average	1–1000 km	0–60 m	Relatively flat	0.75	1.5	Gaussian model used for receptors out to 50 km
CTDMPLUS[f]	12 to 72 hour	1 km	—	Complex terrain	1.6	2.5	EPA complex terrain model

a Rood (1997).

b Ramsdell et al. (1994).

c Miller and Hively (1987).

d Robertson and Barry (1989).

e Simpson et al. (1990).

f Genikhovich and Schiermeier (1995).

An additional study (Carhart et al. 1989) not reported in Table 7 included puff dispersion models that were similar to RATCHET (MESOPUFF, MESOPLUME). Evaluations were performed using tracer data bases from Oklahoma and the Savannah River Site. Oklahoma data consisted of two experiments measured at 100 and 600-km arcs downwind of a 3-hour perfluorocarbon release. The Savannah River data involved 15 separate experiments, 2 to 5 days in duration, where ^{85}Kr was released from a 61-m stack and measured at points 28 to 144-km downwind from the source. The ratio of the *average* predicted concentration to the *average*

observed concentration was between 0.5 and 2. Note that this measure is different than the distribution of individual predicted-to-observed ratios reported in Table 7. There was also a tendency for models to overpredict concentrations in both data sets.

The study considered most relevant to the assessment question involved the RATCHET model using the Winter Validation Tracer Study data set. While it is true the release conditions for this study differed from those modeled (i.e., point source and area source) and the averaging time differed (i.e., annual average as opposed to 9-hour average), these data were obtained in the same environs that we are attempting to simulate. In addition, impacts on predicted and observed concentrations because of specific release conditions tend to diminish with increasing receptor distance. Release heights are not that much different from the Winter Validation Tracer Study in which the tracer was released at 10 m above ground level. Abbott and Rood (1996) also showed that the difference between a point and a 100-m diameter area source (represented by a series of point sources distributed in a circular area) released from a height of 0–19 m is at most 5% along the plume centerline at a distance of 2 km or greater for all combinations of wind speed and stability. We conclude that the major difference between the Winter Validation Data set and our current situation resides with the averaging time.

The largest range of predicted-to-observed ratios reported in Table 7 involved complex terrain, which suggests models are more sensitive to the local meteorological and terrain conditions than other factors such as release height. For example, note the geometric standard deviation (GSD) for short-term estimates using the Gaussian plume model at a highly instrumented site for elevated source increases by about 9% from its ground-level counterpart but the difference between the GSD for flat and complex terrain is almost an order of magnitude.

With the distribution of predicted-to-observed ratios for RATCHET from the Winter Validation Tracer Study as our starting point, our approach was to modify this distribution based on (a) the differences between the study conditions and those of past releases, and (b) our assessment question (i.e., What is the annual average concentration for each year of the assessment period?). We combined data points at the 8 and 16 km distance into a composite set and justified this action based on the evaluations in Rood (1997) that showed similar geometric mean (GM) and GSD values for 8 and 16-km data. In addition, the confidence intervals on the GM and variance of the observed-to-predicted ratio overlapped. The composite distribution had a GM of 0.95 and GSD of 4.4. Predicted-to-observed ratios are plotted as a function of the number of standard deviations from the mean (normalized to the standard normal distribution) in Figure 5. Note that most of the data points ($\pm 2\sigma$) lie along the line representing the lognormal fit to the data, with the exception of the tails. We, therefore, represent the distribution of predicted-to-observed ratios as a lognormal distribution with a GM and GSD as defined above. Points on the tails, particularly those with predicted-to-observed ratios less than 0.01, were associated with Test 5 (February 9, 1991) at the 8-km arc in the east–northeast sector for the hours 16:00 to 18:00. All models performed poorly for this test. Concentrations in east–northeast sector were grossly underestimated (greater than a factor of 10 difference), and the ground-level contaminant mass at 8 km was also underestimated. Models appeared to have difficulty responding to the transition from daytime to nighttime stability conditions. During the latter hours of the test and under predominately nighttime conditions (18:00–23:00), predicted concentrations showed better agreement with the observations.

As stated previously, the major difference between the Winter Validation Tracer Study data and the assessment question is the averaging time. Averaging time appears to have a large impact

on the range of predicted-to-observed ratios encountered. For example, Simpson et al. (1990) reports the GSD of the predicted-to-observed ratio is reduced 38% with an increase in averaging time from 12 to 72 hours (Table 7). Also note the GSD for the annual average and short-term predicted-to-observed ratio for the Gaussian plume model under complex terrain conditions increases from 3.8 to 14. Validation exercises performed with RATCHET at the Hanford Reservation for an elevated release at distances greater than 20 km showed a slight overprediction by the model (GM = 1.4) and a GSD value of 2.2, which is about 50% smaller than the GSD for the Winter Validation Tracer Study data. It is not clear whether these differences are due to averaging time, release height, terrain conditions, or receptor distance, but based on the other studies reviewed in Table 7, it is likely that the smaller GSD is primarily due to increased averaging time.

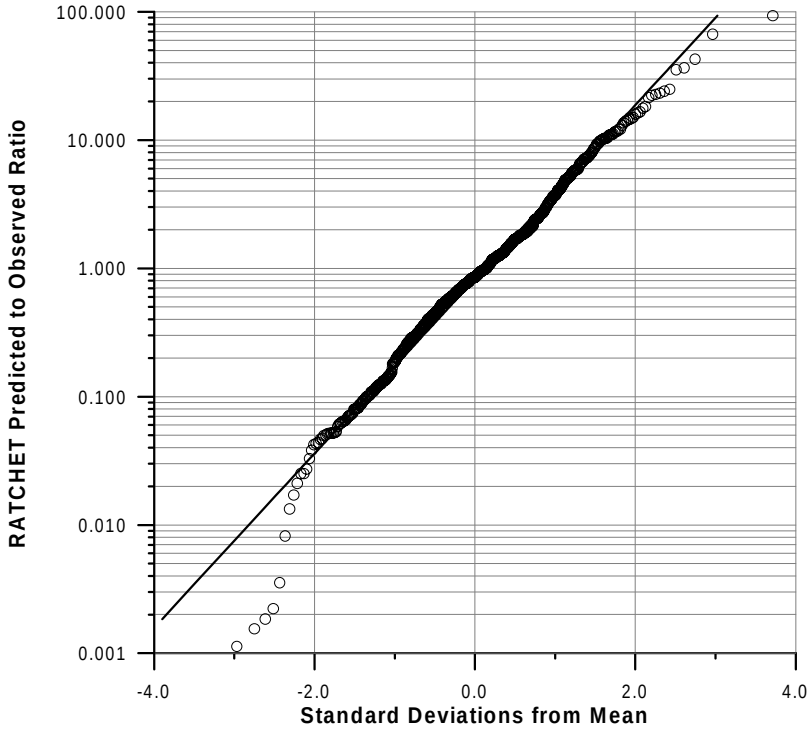

Figure 5. Predicted-to-observed ratios for the RATCHET model as a function of standard deviation from the mean (normalized to a mean of 0 and standard deviation of 1). The solid line represents the lognormal fit to the distribution. Circles represent individual data points.

Key observations relevant to defining the distribution of the correction factor are summarized as follows.

- GSD of predicted-to-observed ratios decreases with increasing averaging time
- GSD of predicted-to-observed ratios increases with increasing terrain complexity
- GSD of predicted-to-observed ratios increases for receptor distances >10-km
- GM of the predicted-to-observed ratio is greater than 1.0 for receptor distances >20 km.

The GSD is expected to fall somewhere between 1.2 and 4.4 based on the data in Table 7. Noting the key observations stated above and the data in Table 7, the following values for GM and GSD were assigned to the predicted-to-observed ratio

- GSD = 2.2 and GM = 0.95 for receptors <8 km
- GSD = 2.0 and GM = 0.95 for receptors >8 km and <16 km
- GSD = 2.2 and GM = 1.0 for receptors >16 km.

The distribution of predicted-to-observed ratios translate into dispersion correction factors listed in Table 9 in the summary section. The GSD value of 2.2 was the same value calculated for monthly averages using RATCHET at the Hanford Reservation. It may be argued that a lower value is more appropriate because the averaging time is longer. We have chosen this value because the GSD of monthly average predicted-to-observed ratios will likely be higher for Rocky Flats compared to Hanford because of terrain complexities. In addition, no annual average predicted-to-observed ratios exist for the Rocky Flats environs. Therefore, uncertainty bounds should be kept large to account for our lack of knowledge. Adjustments in the GSD and GM were also made to account for receptor distance. The GSD was reduced from 2.2 to 2.0 for receptors 8 to 16 km from RFP because the Winter Validation Tracer Study measurements were made at these distances and the lower value reflects our greater confidence in uncertainty at these distances. The GM was held at the same value calculated with the Winter Validation Tracer Study data for receptor distances <16 km and increased to 1.0 for receptor distances >16 km. The GM value was increased to reflect the tendency for models to overpredict at greater distances. Validation studies indicate predicted-to-observed ratios greater than 1.0 (reflecting model overprediction) at distances greater than 20 km. While this may be true, we have no site-specific data to verify this observation for our model domain. The lower GM predicted-to-observed ratio will potentially result in model overprediction and, thereby, provide at least a conservative estimate of concentrations at these distances. Correction factor distributions were truncated by a minimum value of 0.01 and a maximum of 1000.

Application of this factor on a year-by-year basis assumes year-to-year annual average concentrations are independent from one another. Analysis of the annual average X/Q values for each year in the 5-year meteorological data set indicated annual average concentrations at some locations are correlated (to some degree) from year-to-year. Ideally, we would like to have meteorological data from the entire assessment period in order to estimate the year-to-year correlations, but these data are lacking. To account for the unknown year-to-year correlation, we have assumed a correlation coefficient of 1.0. This assumption will tend to overestimate uncertainty in time-integrated concentration (*TIC*), but is justified based on our lack of knowledge about year-to-year correlations. Details concerning incorporation of this factor in the Monte Carlo uncertainty analysis are discussed in the Risk Calculation section of this report.

Meteorology Uncertainty. Meteorology uncertainty arises because we are using 5 years of meteorological data spanning a recent time period (1989–1993) to define an annual average X/Q value (concentration divided by release rate) that will be applied to all previous years of the assessment period (1952–1989). The question is, how well does this 5-year period represent the past? Comparisons of annual average X/Q values computed with a 5-year data set to the annual average X/Q values computed using the meteorological data for each specific year was recently performed for the Fernald Dosimetry Reconstruction Project (Killough et al. 1996). Meteorological data from the Cincinnati Airport from 1987 to 1991 composed the 5-year composite meteorological data set. Annual average X/Q values computed with these data were

then compared with the annual average *X/Q* value computed for each specific year using the meteorological data for that specific year. The years spanned from 1951 to 1991. Concentrations were calculated at 160 receptors ranging in distance from 1000 to 10,000 m from the release point. A straight line Gaussian plume model for a 10-m release height was used to generate the *X/Q* values. The 5-year composite *X/Q* divided by the *X/Q* for the specific year (P/O ratio) forms the basis of Figure 6 (upper graph). A similar procedure was applied to the *X/Q* values generated for this study and is depicted in the lower graph in Figure 6. However, only the composite period is shown because meteorological data from previous years were not obtained. The lower graph in Figure 6 was generated using the RATCHET model and Building 776 *X/Q* values for 2,300 receptors in the model domain Figure 6 depicts the 5^{th}, 50^{th} and 95^{th} percentile of the cumulative frequency distribution for all points in the model domain. Note that for the composite period, the spread of the data is similar for both data sets.

As one would expect, the spread is much larger for those years that do not include the 5-year composite data. The long-term trend of these data may not depend strongly on location. If this procedure is applied to the RFP environs using Denver Stapleton International Airport data for instance, the locus of the 50^{th} percentiles is likely to look somewhat different, although the amplitudes may be similar. Obtaining meteorological data from past years (1952–1989) for Denver Stapleton International Airport and performing the calculations is not a trivial task, and the overall impact on the results may be similar to what is observed at Cincinnati based on a similar spread of these data for the composite period at both locations. For this reason, we have chosen instead to adapt these data to our analysis.

The Fernald data were represented by a multiplicative correction factor having a GM of 1.0 and GSD of 1.7. This distribution was developed using the following sampling scheme:

1. Noting from Figure 6 that the maximum range in the GMs is a factor of two, a GM was randomly selected from a log-uniform distribution with a minimum $2^{-1/2}$ (0.7) and maximum $2^{1/2}$ (1.4).
2. Using the GM from step (1) and GSD = 1.61 (the maximum GSD calculated from the ratio of the 5-year composite *X/Q* to specific year *X/Q* for the 40 years of data), a sample is drawn from a lognormal distribution with these parameters
3. Values are stored from step (2) and the process is repeated.

This somewhat conservative procedure takes account of the year-to-year variability in the GM of the 5-year composite *X/Q* to specific year *X/Q* ratio, as well as the uncertainty associated with distance and direction from the source. For a sample size of 1000, a lognormal distribution was fitted with a GM = 1.0 and GSD = 1.7.

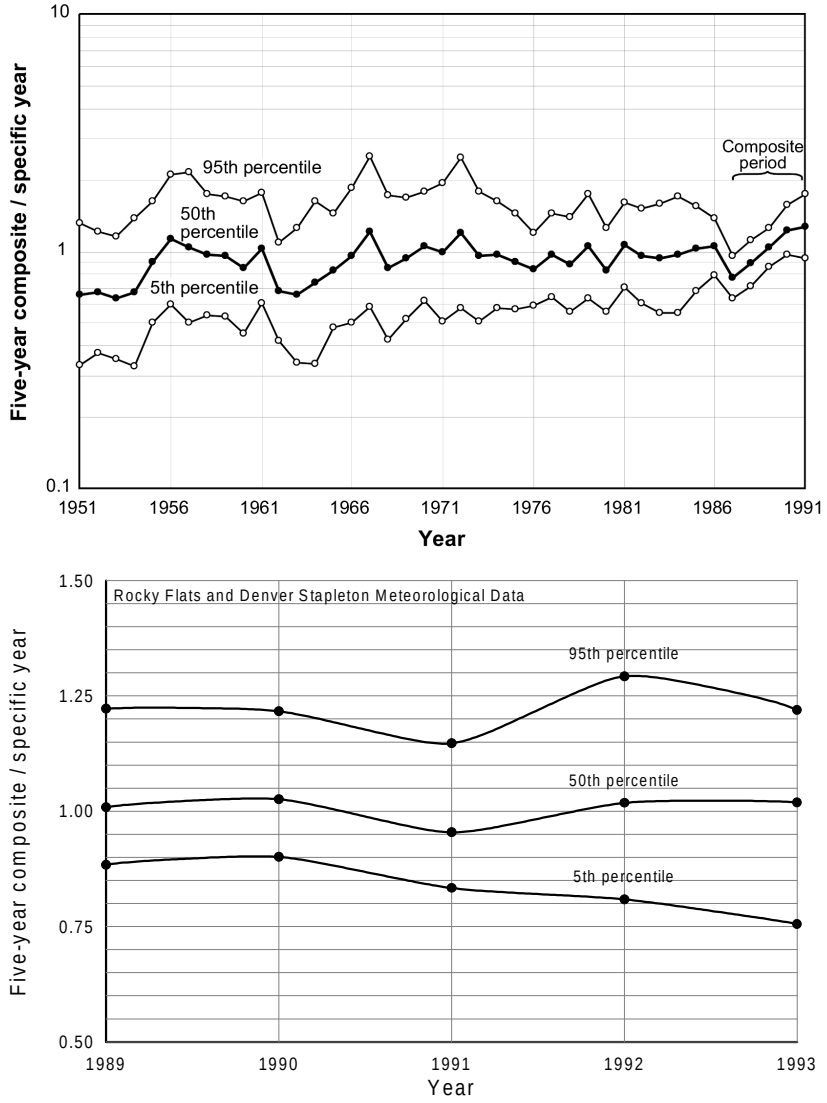

Figure 6. Distributions of P/O ratios for *X/Q* calculated with the Cincinnati meteorological data (upper graph) and RFP–Denver Stapleton International Airport meteorological data (lower graph). Predicted (P) corresponds to *X/Q* values for a five-year composite; observed (O) corresponds to the *X/Q* values for a specific year (from Killough et al. 1996).

Plume Depletion Uncertainty. One factor not considered in many of the field studies was plume depletion from dry deposition. Most field studies use inert tracers to avoid additional complications involving plume depletion and deposition. Miller et al. (1978) illustrates that plume depletion via dry deposition has little impact on inhalation dose for deposition velocities less than 1.0 cm s^{-1} and release heights greater than 50 m for receptors within 10 km of the release point. For ground-level releases, plume depletion has a greater effect. The ratio of the

depleted to non-depleted plume was 0.02 for deposition velocities in the 1.0 cm s^{-1} range and 0.67 for deposition velocities in the 0.1 cm s^{-1} range at a distance of 10-km from the source. Carbon tetrachloride was not released at ground level or at 50 m, and deposition velocities calculated in RATCHET ranged from 0.3 to 1.0 cm s^{-1}. Therefore, the actual amount of plume depletion would be somewhere between these values. Deposition velocities in the 1.0 cm s^{-1} range are associated with roughness lengths of around 2.0 m, which are limited to the foothills region of the model domain where few receptors are present. For these reasons, the uncertainty in the predicted concentration from plume depletion and deposition is expected to be small for most receptors in the model domain.

Deposition velocity is not an input parameter in RATCHET, but it is calculated (using Equations [2–5]) for each hour of the simulation. Deposition velocity is a function of the frictional velocity, wind speed, and a user defined transfer resistance (r_t). The frictional velocity (Equation [5]) is a function of wind speed, roughness height, and a stability correction factor that is a function of the Monin-Obukhov length and wind speed measurement height. Our approach is to vary the Monin-Obukhov length and transfer resistance and calculate alternative values for deposition velocity for a given wind speed and stability classification. Airborne concentrations calculated with alternative values for deposition velocity are compared to the airborne concentrations of the base case. The base case concentrations represent model predictions made using a transfer resistance of 100 s m^{-1} and a Monin-Obukhov length that represents the mid-range of possible values for a given stability class. (RATCHET uses the mid-range of the possible Monin-Obukhov lengths for a given stability class when run in a deterministic mode.)

The random sampling feature in RATCHET was used to vary the Monin-Obukhov length. When random sampling is selected, specific values of the inverse Monin-Obukhov length are obtained from the range of Monin-Obukhov lengths for a given stability class. A random value between 0 and 1 is obtained and used to calculate a value of the inverse Monin-Obukhov length assuming that the inverse Monin-Obukhov length is uniformly distributed within the range.

Distributions of the transfer resistance must be provided outside the RATCHET code. The rational for the distribution of r_t was based the distribution of deposition velocities reported in Harper et al. (1995). The 5^{th}, 50^{th}, and 95^{th} percentile values for deposition velocity of a 1 μm particles and 5 m s^{-1} wind speed were 0.01, 0.21, and 4.1 cm s^{-1} respectively. Assuming a lognormal distribution and a 50^{th} percentile r_t value of 100 s m^{-1}, we multiply the ratio of the $5^{th}/50^{th}$ percentile and $95^{th}/50^{th}$ percentile from the distribution of deposition velocities by the 50^{th} percentile transfer resistance value. The 5^{th} percentile for the distribution of r_t was 0.01/0.21 × 100 s m^{-1} = 4.8 s m^{-1}. The 95^{th} percentile for the distribution of r_t was 4.1/0.21 × 100 s m^{-1} = 1952 s m^{-1}. A distribution containing 100 individual r_t values was generated in Crystal Ball and output to an ASCII file to be used in the uncertainty simulation. The corresponding 5^{th} and 95^{th} percentile deposition velocity calculated using a 5 m s^{-1} wind speed, roughness lengths from 0.001 to 2.0 m, and the mid-range value for the Monin-Obukhov length, was 0.05 and 1.5 cm s^{-1}, respectively. The range of deposition velocities used in RATCHET simulations would be greater because the Monin-Obukhov length is also varied.

A shell program was written to facilitate the plume depletion uncertainty calculations. For each trial, a value of r_t was read from the distribution file created earlier and written to the RATCHET input file. The RATCHET code was then called from the shell program and run using meteorological data spanning 1 year (1990) and a unit release rate. Concentrations were output for 156 receptors located 1 to 32 km from the source. Output concentrations were saved

and the process was repeated until all 100 r_t values were run. A correction factor was calculated for each trial and each receptor. The correction factor is given by

$$CF_{i,j} = \frac{C_{i,j}}{Cb_j} \tag{10}$$

where $CF_{i,j}$ = the correction factor for i^{th} trial and j^{th} receptor, $C_{i,j}$ = the concentration calculated for the i^{th} trial and j^{th} receptor, and Cb_j = the base case concentration for the j^{th} receptor. Correction factors were segregated into bins according to receptor distance. The GM and GSD were then calculated for all CF values within a given bin (Table 8).

Table 8. Plume Depletion Uncertainty Correction Factors

Distance (km)	GM	GSD
4	0.99	1.05
8	1.00	1.09
12	1.01	1.12
16	1.00	1.14
20	1.00	1.16
24	1.00	1.17
28	1.01	1.18
32	1.01	1.18

These data show a GM near 1.0 and a GSD that increases as a function of receptor distance. As expected, the uncertainty is small, especially near the source, but uncertainty increases at greater receptor distances. The plume depletion uncertainty correction factor was assigned a lognormal distribution with a GM of 1.0 and a GSD that varies with receptor distance as given in Table 8.

Summary of Prediction Uncertainty. Three correction factors are applied to our model predictions. The first correction factor accounts for the uncertainty associated with the prediction of the annual average concentration for a specific year assuming we have the meteorological data for that year. The second correction factor accounts for the uncertainty associated with using a 5-year composite meteorological data set (1989–1993) to predict the annual average concentration for years past (1953–1989). The third correction factor accounts for uncertainty in the dry deposition rate and resulting plume depletion. The three correction factors are independent of one another and are represented by lognormal distributions. The dispersion correction factor is assumed to be correlated from year to year (correlation coefficient = 1.0). The other correction factors are independent from year-to-year. Table 9 summarizes all three correction factors. Integration of these stochastic factors into the *TIC* estimates are discussed in the Risk Calculations section of this report.

Table 9. Summary of Uncertainty Correction Factors Applied to Annual Average Concentration Predictions

Receptor distance	Dispersion uncertainty		Meteorology uncertainty		Depletion uncertainty	
(km)	GM[a]	GSD	GM	GSD	GM	GSD
<4	1.1	2.2	1.0	1.7	1.0	1.05
8	1.1	2.0	1.0	1.7	1.0	1.09
12	1.1	2.0	1.0	1.7	1.0	1.12
16	1.1	2.0	1.0	1.7	1.0	1.14
20	1.0	2.2	1.0	1.7	1.0	1.16
24	1.0	2.2	1.0	1.7	1.0	1.17
28	1.0	2.2	1.0	1.7	1.0	1.18
>32	1.0	2.2	1.0	1.7	1.0	1.18

[a] Dispersion uncertainty GM is the inverse of the GM of predicted-to-observed ratios.

Annual Average *X*/*Q* Values

The procedure and models described in the previous sections were used to calculate an annual average *X*/*Q* for all concentration grid nodes in the model domain. Grid node spacing for the concentration grid was set at 1000 m. The annual average *X*/*Q* at each of the grid nodes for each year of meteorological data (1989–1993) was computed for a constant unit release (1 μg s^{-1}). The five *X*/*Q* values at each grid node were then averaged to yield a 5-year composite annual average *X*/*Q*. The maximum *X*/*Q* in the model domain of 6.3×10^{-6} s m^{-3} was estimated to occur within the confines of the plant near Building 776. Isopleth maps were generated using *X*/*Q* data gridded using the minimum curvature routine found in the Surfer® software (Golden Software Inc. 1996).

The dispersion patterns shown in Figure 7 are characterized by a east-northeast trending ellipsoid shaped plume. Wind roses constructed using RFP data from 1984–1993 (DOE 1995) indicate the predominant wind direction to be from the west northwest. Higher concentration isopleths near the source trend mostly easterly; however, farther away from the source, concentration isopleths trend to the northeast. The northeast trend is believed to be due to the influence of the Platte River Valley and the diurnal pattern of upslope-downslope conditions that characterize the general air movement on the Colorado Front Range environs (Crow 1974). Downslope conditions typically occur during the evening hours and are characterized by drainage flow of cooler air from the foothills to the plains. Westerly winds predominate, but the direction may be altered by local topography. Upslope conditions are a result of daytime heating and typically result in easterly winds that prevail during the daylight hours with transition from upslope to downslope conditions occurring during the evening and transition from downslope to upslope occurring during the morning. During evening hours under stable conditions, cool air near the surface drains from the Denver metropolitan area down the Platte River Valley (which flows to the northeast) and out to the plains. During daylight hours and after surface heating has eliminated the cooler surface layer, the downslope conditions cease. This is followed by a brief period of relatively calm winds, which in turn is followed by return of air up the valley or

upslope conditions. Meteorological data at Denver Stapleton International Airport captures these transitions in the Platte River Valley that are reflected in the *X*/*Q* isopleth maps.

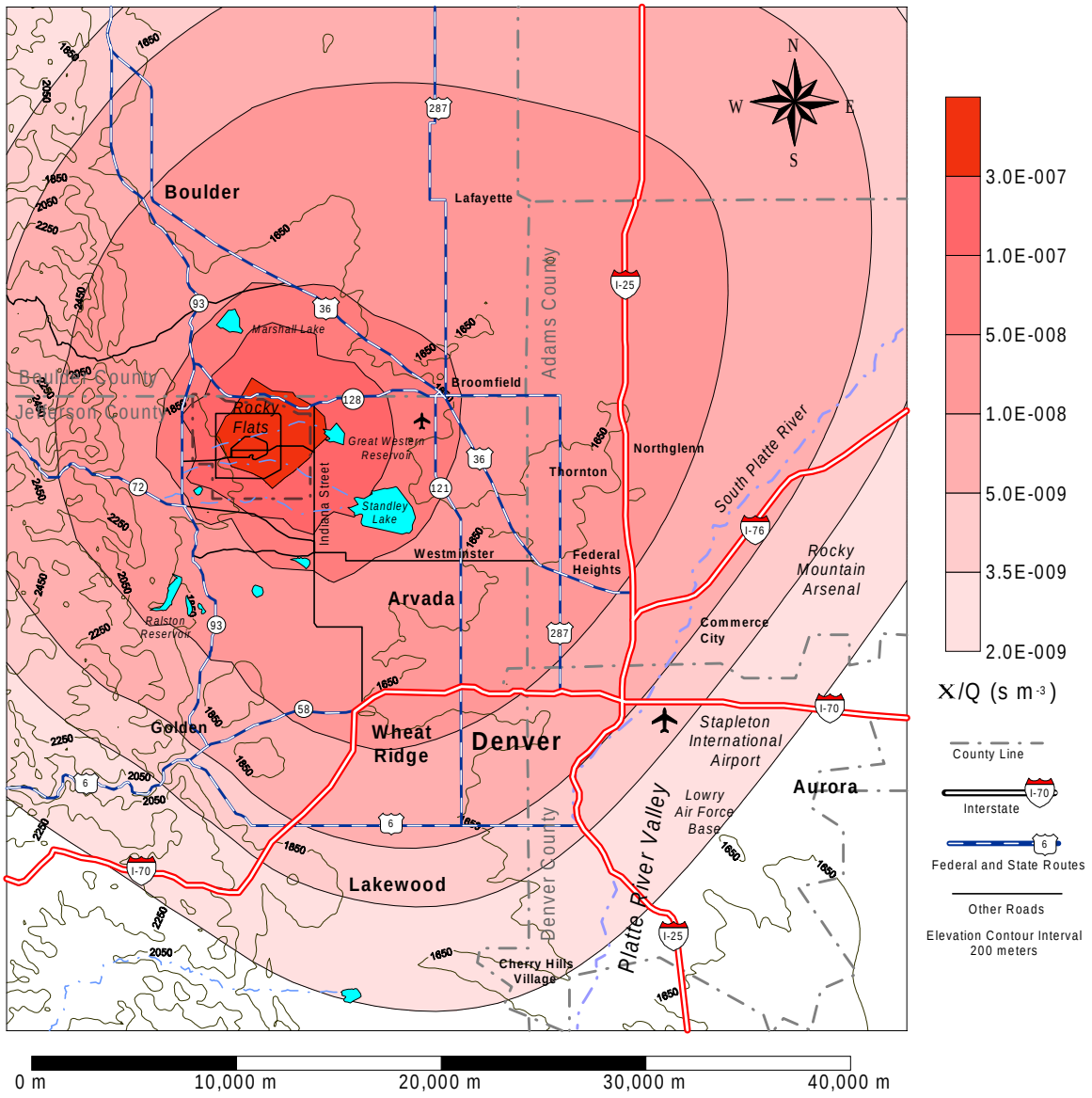

Figure 7. Isopleth map of the annual average X/Q for gaseous releases from Building 776 using meteorological data from the RFP and Denver Stapleton International Airport from 1989–1993.

Predicted Concentrations

Predicted concentrations of carbon tetrachloride at specific receptor locations were calculated for each year that source term information was available. Uncertainty in the predicted concentration included uncertainty in the dispersion estimate and source term. The concentration at a given location for the i^{th} year was given by

$$C_i = \frac{\chi}{Q} Q_i \; CF_1 \; CF_2 \; CF_3 \qquad (11)$$

where
Q_i = annual release of carbon tetrachloride for the i^{th} year
CF_1 = dispersion uncertainty correction factor
CF_2 = meteorology uncertainty correction factor
CF_3 = plume depletion uncertainty correction factor.

The correction factors and source term (Q_i) are stochastic quantities. Therefore, the concentration is also a stochastic quantity. Figure 8 depicts the predicted concentration east of the plant along Indiana Street (the location of highest concentration outside the buffer zone) as a function of time. Note that the median value (50th percentile) estimated concentrations are about the same as background (1 µg m–3) for the years 1958–1973.

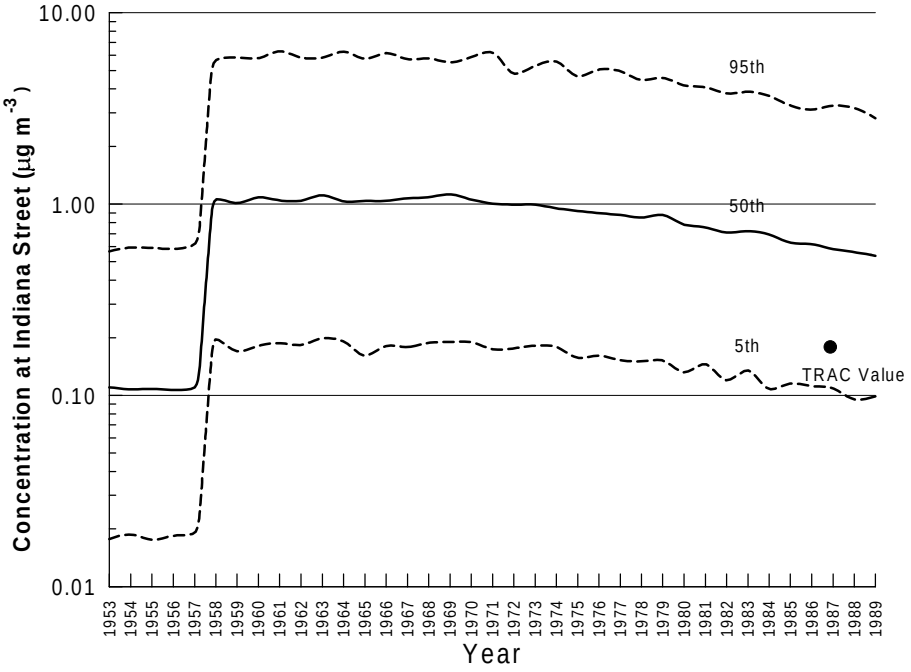

Figure 8. Predicted carbon tetrachloride concentration as a function of year for a receptor located east of the plant on Indiana Street. The three lines represent the 5th, 50th, and 95th percentiles on the cumulative density function. The point labeled TRAC value was the annual average concentration estimated for 1988 using the TRAC model.

Time-integrated concentrations were calculated on a receptor-specific basis. Concentrations were integrated over the duration of time the receptor resided in a given location in the model domain and are reported in the Exposure Scenario and Risk Calculation section of the report.

Unfortunately, limited ambient air monitoring of carbon tetrachloride was performed during the assessment period, so validation of predicted concentrations is difficult at best. Lugar (1990) reported measurements of carbon tetrachloride made on June 25, 28, and July 13, 1989. Measurements were made at 4 locations surrounding the facility at the edge of the buffer zone.

Comparisons of these measurements with predicted values were performed by Rood (1997) and presented in Appendix A. Comparisons represent a qualitative evaluation because the carbon tetrachloride source term for the days measurements were made was unknown.

Other past modeling studies (Rockwell 1989) used the TRAC model to predict annual average concentrations of carbon tetrachloride for releases that occurred in 1988. The source term used in these simulations originated from the SARA Title III emissions inventory for Rocky Flats. The emission rate used in the TRAC simulation was not reported in the document and it is unknown how it compares with the estimates used in this study. All emissions were assumed to come from Building 776. Meteorological data included 1-year of data (1983) taken at the RFP and Denver Stapleton. The document states the meteorological data were inappropriate for a comprehensive study, but judged these data adequate for a preliminary assessment of carbon tetrachloride. The predicted maximum concentration along Indiana Street for 1988 was 0.19 μg m^{-3}. Concentrations for 1988 predicted with RATCHET and our estimated emission rate ranged from 0.095 (5^{th} percentile) to 3.2 μg m^{-3} (95^{th} percentile). It is difficult to state if any one model is over or underpredicting relative to one another without knowing the source term used in the TRAC analysis. However, it does provide some outside verification that the concentration estimates made by the RATCHET model are in the range of values predicted by other models and investigators.

EXPOSURE SCENARIOS AND RISK CALCULATIONS

One of the key parts of the Rocky Flats Dose Reconstruction work is calculating health impacts to people living in the surrounding area from materials released during RFP past operations. Dose reconstruction uses a pathways approach to study the potential radiation doses and health risks of these past releases on the surrounding communities. The pathways approach begins with learning what kinds of and how much materials were released from a facility and ends with estimating the health impacts these releases had on the residents in the area. Mathematical models described in the previous section were used to model the transport of materials released from the site to the surrounding communities. In this section, we calculate health impacts (lifetime cancer incidence risk) to people living offsite from exposure to these releases.

Clearly, at this point in the study, it is not realistic to calculate individual risks for every resident who may have lived or worked in the Rocky Flats area during its operational history. At the other extreme, it is not credible to calculate only a single risk that would apply to all residents. The risk that a person receives depends upon a number of factors, such as

- Lifestyle (that is, did the person spend a great deal of time outdoors or doing heavy work on a farm)
- When and how long that person lived near the RFP (for example, during the key release events in 1957 and late 1960s or in the 1970s when releases were less)
- Age and gender of the person
- Where the person lived and worked in relation to the RFP.

To consider these features of a person's life, we developed profiles, or exposure scenarios, of hypothetical, but typical residents of the RFP area for which representative risk estimates could be made. Each scenario represents one individual. These scenarios incorporate typical lifestyles,

ages, genders, and lengths of time in the area. The scenarios can also specify and vary the home and work locations. These scenarios can help individuals determine risk ranges for themselves by finding a lifestyle profile that most closely matches their background. The scenarios are not designed to include all conceivable lifestyles of residents who lived in this region during the time of the RFP operations. Rather, they provide a range of potential profiles of people in the area.

We calculated risks from historical carbon tetrachloride releases from the RFP for nine hypothetical exposure scenarios (Table 10). As discussed earlier, inhalation was the only pathway of exposure considered in the assessment. The residence time of carbon tetrachloride in surface water and soil is relatively short because of its high vapor pressure and volatility. Therefore, concentrations in these media are expected to be inconsequential compared to concentrations in the ambient air.

Exposure scenarios for the nine hypothetical receptors described in Table 10 were organized according to occupational and nonoccupational activities. Occupational activities include work, school, and extracurricular activities away from the home. Nonoccupational activities include time spent at home doing chores, sleeping, and leisure activities such as watching television. For some scenarios, the receptor was assumed to perform occupational and nonoccupational activities at a different location. For example, the office worker lives in Broomfield but works in downtown Denver. The age of the receptor and years during which exposure occurred are also considered in the when calculating exposures. The last three exposure scenarios represent the same individual but at different periods in their life. Cumulative risks over this receptor's lifetime are also reported.

Breathing Rates and Time Budgets

Each exposure scenario was divided into three types of activities: sleeping, nonoccupational activity, and occupational activity. For the infant and child scenario, occupational and nonoccupational activities are irrelevant, so instead, activities were divided into sleeping and two other activities based on the child's age. For the infant, the other two activities were awake sedentary and awake active. For the child scenario, time spent at home (indoors and outdoors) and time spent at preschool and or day care were the other two activities.

For each activity, time spent at four different exercise levels were assigned. These exercise levels were resting, sitting (sedentary), light exercise, and heavy exercise. Some examples of light exercise are laboratory work, woodworking, housecleaning, and painting. Heavy exercise usually does not exceed 2 hours per day and corresponds to occupations such as mining, construction, farming, and ranching. For each exercise level, an age- and gender-specific breathing rate was assigned. Breathing rates (Table 11) for persons age 8 and higher were obtained from Roy and Courtay (1991) and from Layton (1993) for children age 0–7.

Table 10. Exposure Scenario Descriptions

Exposure scenario	Sex	Year of birth	Year beginning exposure	Year ending exposure	Location of occupational activities	Location of nonoccupational activities
Rancher	Male	1925	1953	1989	Indiana St.	Indiana St.
Office worker	Female	1951	1975	1989	Denver	Broomfield
Housewife	Female	1928	1953	1989	Broomfield	Broomfield
Retiree	Male	1923	1978	1989	Arvada	Arvada
Laborer #1	Male	1953	1974	1989	Thornton	Commerce City
Laborer #2	Male	1933	1953	1974	Commerce City	Westminster
Infant[a]	Female	1953	1953	1954	Broomfield	Broomfield
Child[a]	Female	1953	1955	1960	Broomfield	Broomfield
Student[a]	Female	1953	1961	1971	Westminster	Broomfield

a. These receptors are the same individual. Total risk over their lifetime is also reported

Table 11. Breathing Rates for Various Exercise Levels as Reported in Roy and Courtay (1991) and Layton (1993)

Gender	Age	Resting ($m^3\ h^{-1}$)	Sitting ($m^3\ h^{-1}$)	Light ($m^3\ h^{-1}$)	Heavy ($m^3\ h^{-1}$)
Male	30-60	0.45	0.54	1.50	3.00
Female	30-60	0.32	0.39	1.26	2.70
Male	18	0.50	0.60	1.58	3.06
Female	18	0.35	0.42	1.32	1.44
Male	16	0.43	0.52	1.52	3.02
Female	16	0.35	0.42	1.30	2.70
Male	15	0.42	0.48	1.38	2.92
Female	15	0.35	0.40	1.30	2.57
Male	14	0.41	0.49	1.40	2.71
Female	14	0.33	0.40	1.20	2.52
Male	12	0.38	0.47	1.23	2.42
Female	12	0.33	0.39	1.13	2.17
Male	10	0.31	0.38	1.12	2.22
Female	10	0.31	0.38	1.12	1.84
Male	8	0.29	0.39	1.02	1.68
Female	8	0.29	0.39	1.02	1.68
Male	3-7	0.24	0.29	0.72	1.68
Female	3-7	0.23	0.27	0.68	1.59
Male	0-3	0.19	0.23	0.58	1.35
Female	0-3	0.14	0.17	0.45	1.02
Average, male[a]	8–17	0.37	0.45	1.28	1.49
Average, female[a]	8–17	0.33	0.40	1.18	2.25

a The average female breathing rate from age 8–17 was used in Scenario 9

Time budgets for various receptor activities were also based on Roy and Courtay (1991) (Table 12), but they were modified to fit specific exposure scenarios. The fraction of time spent at a specific exercise level while engaged in a given activity was assigned based on the nature of the activity. For example, the fraction of time spent at the resting exercise level while the receptor slept would be 1.0 and the other exercise levels would be 0. A weighted-average breathing rate was then applied to each activity based on the number of hours spent at each exercise level. For some scenarios (housewife, retiree, and laborer), nonoccupational activities were separated into those performed indoors and those performed outdoors. Although no distinction was made between indoor and outdoor air concentrations, exercise levels for indoor and outdoor activities differed. A time-weighted average breathing rate that included indoor and outdoor activities was calculated and applied to nonoccupational time. Each receptor was assumed to spend 15 days per year away from the Denver metropolitan area and outside the model domain. Contaminant concentrations were assumed to be the same for indoor and outdoor air.

Time-weighted average breathing rates were calculated for the three activities for which each receptor was assumed to be engaged. The time-weighted average breathing rate is given by

$$WBR_j = \sum_{i=1}^{4} BR_i \; f_{i,j} \qquad (12)$$

where

WBR_j = time-weighted average breathing rate for the j^{th} activity ($m^3\ h^{-1}$)
BR_i = breathing rate for the i^{th} exercise level ($m^3\ h^{-1}$)
$f_{i,j}$ = fraction of time spent at the i^{th} exercise level for the j^{th} activity.

To reiterate, three activities were defined for each exposure scenario. The location of exposure for occupational activities may be different from nonoccupational activities. The breathing rate during a given activity was the time-weighted average breathing rate of the four exercise levels. Exercise levels were grouped into resting, sitting, light exercise, and heavy exercise.

Risk Calculation and Uncertainty

Calculation of lifetime cancer incidence risk involved three steps:

1. Calculate the *TIC* at the point of exposure.
2. Calculate the amount of carbon tetrachloride inhaled by the receptor.
3. Multiply the carbon tetrachloride intake by a slope factor that relates the risk of cancer incidence to the amount of carbon tetrachloride inhaled per day per unit body weight.

In each of these steps, Monte Carlo sampling techniques are used to propagate uncertainty through the calculation. A Monte Carlo calculation consists of multiple iterations or trials of a computational endpoint (risk). For each trial, parameter values are randomly chosen from distributions that quantitatively describe our knowledge of the parameter. After randomly selecting a set of parameter values, the endpoint is calculated and the procedure is repeated numerous times until an adequate distribution of the endpoint is obtained.

Table 12. Time Budgets, Weighted Breathing Rates, and Body Weights (*BW*)[a] for the Exposure Scenarios

Scenario	Activity	Fraction of time spent at an exercise level				Hours per day (workweek)	Hours per day (weekend)	Hours per year	Weighted breathing rate ($m^3\ h^{-1}$)
		Resting	Sitting	Light	Heavy				
Rancher	Occupational	0.00	0.00	0.25	0.75	8.0	8.0	2800	2.62
(*BW* = 78.7 kg)	Nonoccupational	0.00	0.50	0.38	0.13	8.0	8.0	2800	1.21
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.45
Office worker	Occupational	0.00	0.25	0.75	0.00	8.0	0.0	2000	1.04
(*BW* = 65.4 kg)	Nonoccupational	0.00	0.50	0.38	0.13	8.0	16.0	3600	1.00
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.32
Housewife	Occupational	0.00	0.13	0.75	0.13	8.0	8.0	2800	1.33
(*BW* = 65.4 kg)	Nonoccupational								
	Indoor	0.00	0.50	0.38	0.13	4.0	4.0	1400	1.00
	Outdoor	0.00	0.38	0.50	0.13	4.0	4.0	1400	1.11
	Total nonoccupational	0.00	0.44	0.44	0.13	8.0	8.0	2800	1.06
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.32
Retiree	Occupational	0.00	0.50	0.50	0.00	8.0	8.0	2800	1.02
(*BW* = 78.7 kg)	Nonoccupational								
	Indoor	0.00	0.50	0.38	0.13	6.0	6.0	2100	1.21
	Outdoor	0.00	0.50	0.38	0.13	2.0	2.0	700	1.21
	Total nonoccupational	0.00	0.50	0.38	0.13			2800	1.21
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.45
Laborer #1	Occupational	0.00	0.13	0.50	0.38	8.0	0.0	2000	1.94
(*BW* = 78.7 kg)	Nonoccupational								
	Indoor	0.00	0.50	0.38	0.13	6.0	8.0	2300	1.21
	Outdoor	0.00	0.50	0.25	0.25	2.0	8.0	1300	1.40
	Total nonoccupational	0.00	0.50	0.31	0.19			3600	1.28
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.45
Laborer #2	Occupational	0.00	0.13	0.50	0.38	8.0	0.0	2000	1.94
(*BW* = 78.7 kg)	Nonoccupational								
	Indoor	0.00	0.50	0.38	0.13	6.0	8.0	2300	1.21
	Outdoor	0.00	0.50	0.25	0.25	2.0	8.0	1300	1.40
	Total nonoccupational	0.00	0.50	0.31	0.19			3600	1.28
	Sleeping	1.00	0.00	0.00	0.00	8.0	8.0	2800	0.45
Infant	Awake–sedentary	0.00	0.71	0.14	0.14	7.0	7.0	2450	0.33
(*BW* = 9.4 kg)	Awake –active	0.00	0.00	1.00	0.00	1.0	1.0	350	0.45
	Sleeping	1.00	0.00	0.00	0.00	16.0	16.0	5600	0.14
Child	Home								
(*BW* = 15.8 kg)	Indoor	0.00	0.50	0.42	0.08	6.0	6.0	2100	0.55
	Outdoor	0.00	0.00	0.67	0.33	1.5	1.5	525	1.04
	Total home					7.5	7.5	2625	0.65
	School-indoor	0.00	0.80	0.20	0.00	2.5	2.5	875	0.35
	Sleeping	1.00	0.00	0.00	0.00	14.0	14.0	4900	0.23
Student	Home								
(*BW* = 44.4 kg)	Indoor	0.00	0.44	0.56	0.00	4.5	8.0	1925	0.83
	Outdoor	0.00	0.00	0.25	0.75	2.5	6.0	1225	1.98
	Total home	0.00	0.22	0.40	0.38	7.0	14.0	3150	1.28
	School								
	Indoor	0.00	0.75	0.25	0.00	6.0	0.0	1500	0.59
	Outdoor	0.00	0.00	0.25	0.75	1.0	0.0	250	1.98
	Total school	0.00	0.38	0.25	0.38	7.0	0.0	1750	0.79
	Sleeping	1.00	0.00	0.00	0.00	10.0	10.0	3500	0.33

[a] Body weights were obtained from Finley et al. 1994.

Uncertainty in risk estimates were based on uncertainty in the *TIC* and carcinogenic slope factors. Receptor behavior patterns (i.e., the time spent doing different activities at different exertion levels) and their physical attributes (body weight and breathing rate) were considered fixed quantities. The exposure scenarios were set up to evaluate risks for hypothetical individuals and did not consider variability within the population of potential receptors. Therefore, the parameters describing their physical attributes and behavior were considered fixed.

The procedure outlined above requires an estimate of the *TIC* at the point of exposure. A receptor can be exposed at two locations; place of work (occupational) and place of residence (nonoccupational and sleeping). Consider a Monte Carlo calculation consisting of *m* trials. The *TIC* of the k^{th} trial ($0 < k \leq m$) at location *i* is

$$TIC_i = CF_1 \sum_{l=1}^{n} CF_2 \; CF_3 \; X / Q_i \; Q_l \; \Delta t \qquad (13)$$

where

X/Q_i = dispersion factor for location *i* (y m^{-3})
Q_l = source term for year *l* (mg y^{-1})
CF_1 = stochastic correction factor for dispersion (unitless)
CF_2 = stochastic correction factor meteorology (unitless)
CF_3 = stochastic correction factor for deposition and plume depletion (unitless)
n = number of years exposed
Δt = time increment (1 year).

Notice that the dispersion correction factor (CF_1) is outside the summation symbol. For each Monte Carlo trial, CF_1 is sampled once but the correction factors, CF_2, CF_3, and source term are sampled *n* times. This sampling scheme was used to allow for year-to-year correlation in annual dispersion estimates as discussed earlier. The amount of carbon tetrachloride inhaled by a receptor for the k^{th} Monte Carlo trial is

$$I = TIC_1 WBR_1 T_1 + TIC_2 WBR_2 T_2 + TIC_2 WBR_3 T_3 \qquad (14)$$

where

I = intake of carbon tetrachloride by the receptor for the exposure period (mg)
$TIC_{1,2}$ = time-integrated concentration for occupational and nonoccupational (including sleeping) locations (mg-y m^{-3})
$WBR_{1,2,3}$ = time-weighted average breathing rate for occupational, nonoccupational, and sleeping activity (m^3 h^{-1})
$T_{1,2,3}$ = hours per year for occupational, nonoccupational, and sleeping activity (h y^{-1}).

The subscripts 1, 2, 3 refer to occupational, nonoccupational, and sleeping activity respectively. Note that the *TIC* values (Table 13) are only calculated at two locations and that the same *TIC* value is applied to sleeping and nonoccupational awake activities. Distributions of *TIC* values in Table 13 are described in terms of their *GM* and *GSD*. Analysis of the data points that comprise these distributions show they are best represented by a lognormal distribution. However, in practice, calculations are performed using the actual distribution (made up of *m* number of trials) and not the lognormal representation. Magnitude of the *TIC* was dependent on the length of

exposure, location of exposure, and magnitude of source during exposure. Differences in the GSD values between scenarios are mainly related to the length of exposure and magnitude of the dispersion correction factor. Longer integration time typically corresponds to lower *GSD*s (but not lower variance) because summation of the independent stochastic variables (CF_2 and CF_3) over the integration period results in a lower coefficient of variation (*CV*) of the sum compared to the *CV* of individual years. The *CV* is the standard deviation of the sum divided by the mean of the sum (σ/μ). Like the *CV*, the GSD is a relative measure of the spread of the data comprising the distribution. The decrease in the GSD for longer averaging times is because the *relative* variability in the *TIC* decreases with increasing integration time.

Table 13. Time-Integrated Concentrations for Each Receptor Scenario for Occupational and Nonoccupational Activities

Scenario	Activity	Time-integrated concentration, Building 776[a] (mg-y m^{-3})
Rancher	Occupational	3.5×10^{-2} (2.2)
	Nonoccupational	3.5×10^{-2} (2.2)
Office worker	Occupational	1.4×10^{-4} (2.2)
	Nonoccupational	2.3×10^{-3} (2.0)
Housewife	Occupational	6.4×10^{-3} (2.0)
	Nonoccupational	6.4×10^{-3} (2.0)
Retiree	Occupational	5.4×10^{-4} (2.3)
	Nonoccupational	5.4×10^{-4} (2.3)
Laborer #1	Occupational	7.0×10^{-4} (2.0)
	Nonoccupational	2.4×10^{-4} (2.2)
Laborer #2	Occupational	3.7×10^{-4} (2.2)
	Nonoccupational	2.9×10^{-3} (2.0)
Infant	Occupational	1.9×10^{-5} (2.7)
	Nonoccupational	1.9×10^{-5} (2.7)
Child	Occupational	5.2×10^{-4} (2.2)
	Nonoccupational	5.2×10^{-4} (2.2)
Student	Occupational	1.8×10^{-3} (2.1)
	Nonoccupational	2.5×10^{-3} (2.1)

[a] Geometric mean (geometric standard deviation)

Finally, calculating the incremental lifetime cancer incidence risk requires estimates of the slope factor (SF). The distributions of SFs were reported previously in this report and details are described in Appendix B. Carcinogenic risk from carbon tetrachloride inhalation was calculated using the standard risk equations described in EPA (1989b) and given by Equation 15.

$$R = \frac{SF\ I}{BW\ AT} \tag{15}$$

where

R = incremental lifetime cancer incidence risk
SF = carcinogenic slope factor (kg-d mg^{-1})
I = distribution of integrated contaminant intake (mg)
BW = body mass (kg)
AT = averaging time (70 years × 365 days per year).

Age-specific body weights used in Equation 15 are presented in Table 12. Monte Carlo sampling was performed using a FORTRAN program written specifically for this application. Each step of the Monte Carlo simulation is described below:

1. The distribution of *TIC* values (Equation 13) for each receptor activity and each source were calculated first. Nonoccupational and sleeping activities were assumed to be at the same location. Therefore, 2 *TIC* values were calculated for each receptor. Each *TIC* distribution contained *m* number of individual trials. If occupational and nonoccupational activities occurred at the same location, then a single *TIC* value was used.
2. Each of the *TIC* trials are multiplied by the WBR_i and T_i, (corresponding to the i^{th} receptor activity), then summed over all receptor activities to yield the total contaminant intake of the k^{th} trial (Equation 14). The procedure is repeated for all *m* trials
3. Each estimate of total contaminant intake is multiplied by a randomly selected SF value and divided by body weight and averaging time to give an estimate of the incremental lifetime cancer incidence risk. This calculation is repeated *m* times to yield a distribution of incremental lifetime cancer incidence risks.
4. Percentiles, GM, and GSD values were then calculated from the distribution of *m* risk values.

The total risk over the lifetime of the individual that represents the infant, child, and student scenarios was calculated differently. For each trial, contaminant dose (intake divided by body weight, [mg kg^{-1}]) were calculated for each year the receptor was exposed. Note that body weight and breathing rate change as the individual matures. Meteorological, deposition, and source term uncertainty were applied to each years dose estimate. The dose was summed across all years of exposure then multiplied by the dispersion correction factor and slope factor and divided by the averaging time. This process was repeated *m* times resulting in a distribution of incremental lifetime cancer risk estimates to the individual.

FORTRAN routines for generating random numbers and selecting values from normal, lognormal, triangular, and uniform distributions were adapted from Press et al. (1992). The output distributions provided in this report were generated from 2000 trials.

RISK ESTIMATES

Incremental lifetime cancer incidence risk was greatest for the rancher scenario followed by the housewife, and total child scenarios. Risk estimates were lognormally distributed and described by the GM and GSD for each scenario (Table 14). Appendix C contains detailed output from the computer code used to calculate time-integrated concentrations and risk values. Geometric mean risk values varied from 5.2×10^{-6} for the rancher scenario to 3.4×10^{-9} for the infant. The 5th and 95th percentile values on the cumulative probability function for lifetime risks are shown graphically in Figure 9. Using the rancher scenario as an example, these risks may be interpreted as follows:

- *There is a 90% probability that incremental lifetime cancer incidence risk for the rancher was between 1.3×10^{-6} (5% value) and 2.1×10^{-5} (95% value).*

- *There is a 5% probability that incremental lifetime cancer incidence risk for the rancher was greater than 2.1×10^{-5}.*
- *There is also a 5% probability the risk was less than 1.3×10^{-6}.*

The magnitude of the lifetime risk was dependent on a number of factors, which included duration of exposure, year(s) when exposure occurred, location of exposure, and lifestyle of the receptor. The rancher and housewife scenario had the highest risks; this was primarily due to their close proximity to the RFP (Indiana Street and Broomfield, respectively) and their duration of exposure. The infant scenario had the lowest risk because her duration of exposure was short (1 year) and releases during exposure (1953–1954) were small compared other years. The infant scenario also exhibited the greatest variability (GSD = 2.8). This variability was primarily due to uncertainty associated with the time-integrated concentration and source term.

Also note that the risks for the laborer #2 scenario are substantially higher than those for the laborer #1 scenario. Geometric mean risk for the laborer #1 scenario was 5.1×10^{-8} compared to 2.3×10^{-7} for the laborer #2 scenario. These differences are attributed to the years over which exposure occurred. The exposure period for the laborer #1 receptor was 1974–1989 while the exposure period for the laborer #2 receptor was 1953–1974. Releases during the earlier years of operation (late 50s and 60s) were higher than later years and, therefore, resulted in higher lifetime cancer incidence risks.

Table 14. Incremental Lifetime Carcinogenic Incidence Risk from Carbon Tetrachloride Inhalation Calculated for the Nine Exposure Scenarios

Scenario	GM	GSD
Rancher	5.2×10^{-06}	2.4
Office Worker	1.6×10^{-07}	2.2
Housewife	7.4×10^{-07}	2.2
Retiree	5.0×10^{-08}	2.4
Laborer #1	5.1×10^{-08}	2.3
Laborer #2	2.3×10^{-07}	2.2
Infant	3.4×10^{-09}	2.8
Child	1.0×10^{-07}	2.4
Student	3.5×10^{-07}	2.2
Total (Child)[a]	4.2×10^{-07}	2.4

[a] Total (Child) represents the integrated risk for the infant, child, and student scenarios

There is almost an infinite number of possible exposure scenarios that can be defined, and in most cases, the risks associated with each scenario will differ. However, the risks will probably be bounded by the risks associated with the rancher and infant scenario. The scenario involving the rancher may be considered the maximum exposed individual in the model domain because he was placed at the point of highest concentration outside the RFP buffer zone and remained there for the entire operating period of the plant. However, it is recognized that ranchers could have been grazing cattle within the current buffer zone and up to the old cattle fence. There were also bunkhouses or some type of permanent overnight ranch camp to the northeast within the buffer zone. To increase the risk substantially from our estimates, the concentration within the buffer

zone would have to be several orders of magnitude greater than outside it. This simply is not the case as is evidenced by the *X/Q* plots provided previously in the report. The resulting risk, accounting for occupancy time while exposed to concentrations within the buffer zone, would likely still be in the 10^{-5} to 10^{-7} range.

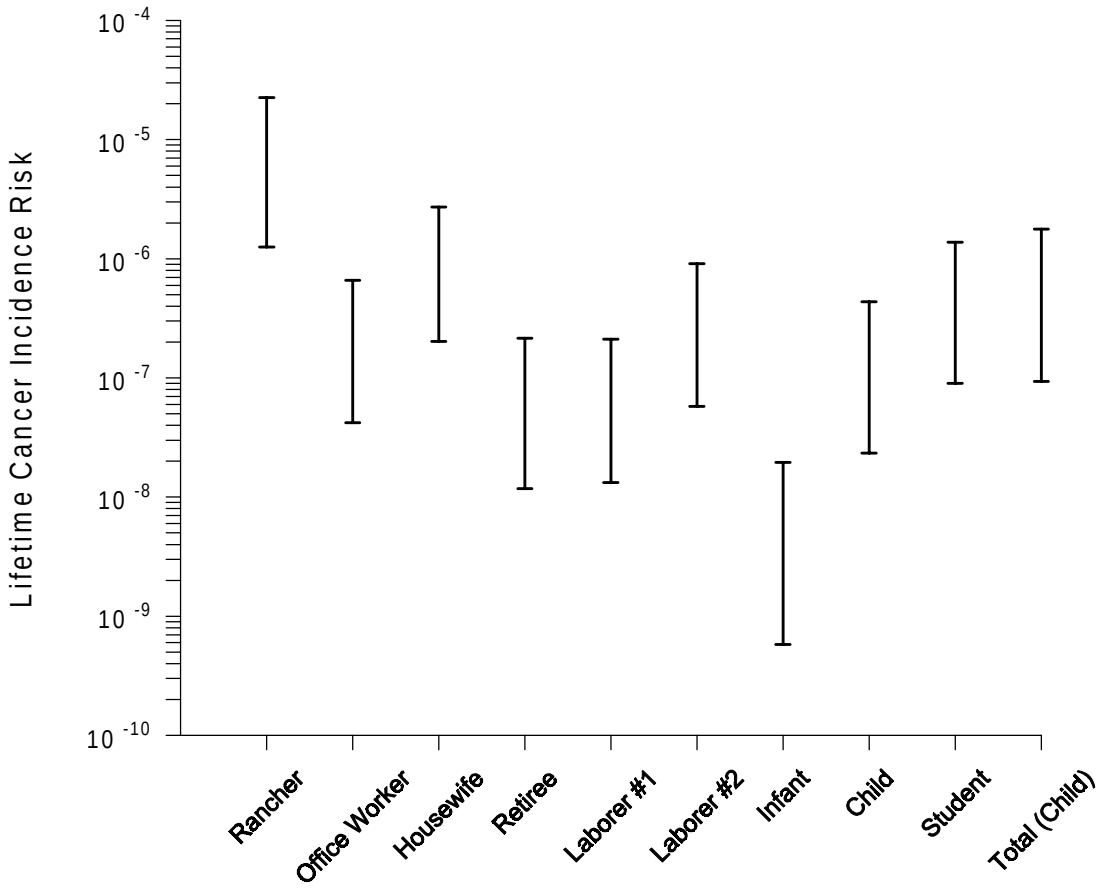

Figure 9. Incremental lifetime cancer incidence risk estimates for the nine exposure scenarios. The range of values shown represent the 5th and 95th percentiles on the cumulative density function. The Total (Child) represents the sum of the infant, child, and student scenarios.

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